

Connecting via Winsock to STN

1/21/01-  
19699106c  
(Part I)  
Structure search

Welcome to STN International! Enter x:x

LOGINID:SSSPTAAJP1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2



\* \* \* \* \* Welcome to STN International \* \* \* \* \*

- NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
- NEWS 2 "Ask CAS" for self-help around the clock
- NEWS 3 SEP 01 New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
- NEWS 4 OCT 28 KOREAPAT now available on STN
- NEWS 5 NOV 30 PHAR reloaded with additional data
- NEWS 6 DEC 01 LISA now available on STN
- NEWS 7 DEC 09 12 databases to be removed from STN on December 31, 2004
- NEWS 8 DEC 15 MEDLINE update schedule for December 2004
- NEWS 9 DEC 17 ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
- NEWS 10 DEC 17 COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
- NEWS 11 DEC 17 SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
- NEWS 12 DEC 17 CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
- NEWS 13 DEC 17 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
- NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN
- NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED
- NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and February 2005
- NEWS 17 JAN 11 CA/CAPLUS - Expanded patent coverage to include Russia (Federal Institute of Industrial Property)
  
- NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
  
- NEWS HOURS STN Operating Hours Plus Help Desk Availability
- NEWS INTER General Internet Information
- NEWS LOGIN Welcome Banner and News Items
- NEWS PHONE Direct Dial and Telecommunication Network Access to STN
- NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 18:24:05 ON 21 JAN 2005

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 18:24:14 ON 21 JAN 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

DICTIONARY FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

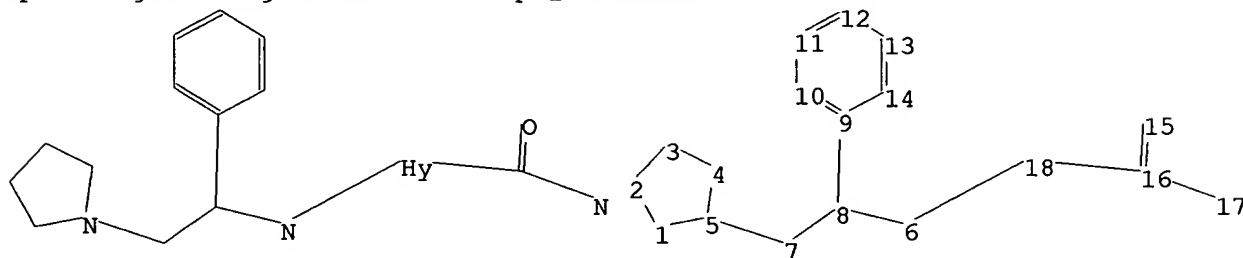
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10699106b.str



chain nodes :

6 7 8 15 16 17 18

ring nodes :

1 2 3 4 5 9 10 11 12 13 14

chain bonds :

5-7 6-8 6-18 7-8 8-9 15-16 16-17 16-18

ring bonds :

1-2 1-5 2-3 3-4 4-5 9-10 9-14 10-11 11-12 12-13 13-14

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 5-7 6-8 6-18 15-16 16-17 16-18

exact bonds :

7-8 8-9

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14

Match level :

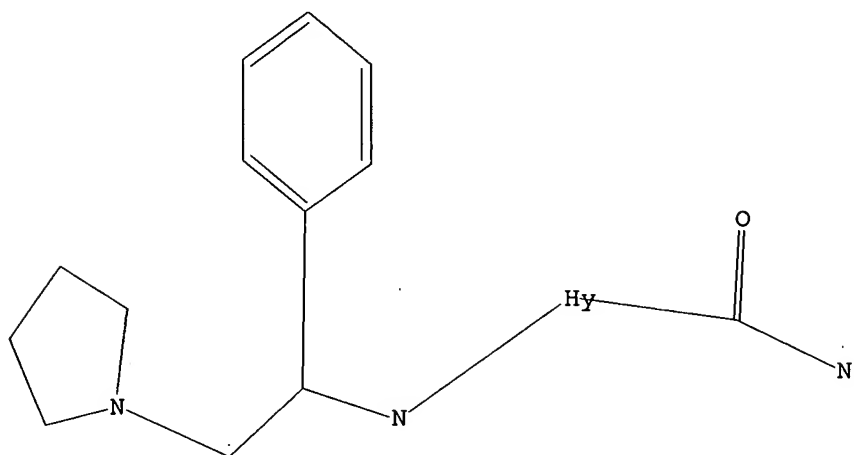
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L1

SAMPLE SEARCH INITIATED 18:24:36 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1356 TO ITERATE

73.7% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 24911 TO 29329

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 18:24:43 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 26680 TO ITERATE

100.0% PROCESSED 26680 ITERATIONS

10 ANSWERS

SEARCH TIME: 00.00.01

L3 10 SEA SSS FUL L1

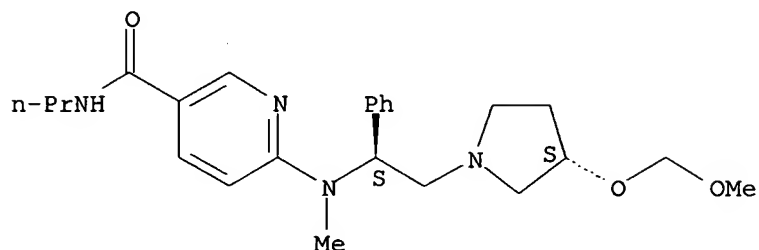
=> d scan

L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 3-Pyridinecarboxamide, 6-[[1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-

1-phenylethyl]methylamino]-N-propyl- (9CI)  
MF C24 H34 N4 O3

Absolute stereochemistry.



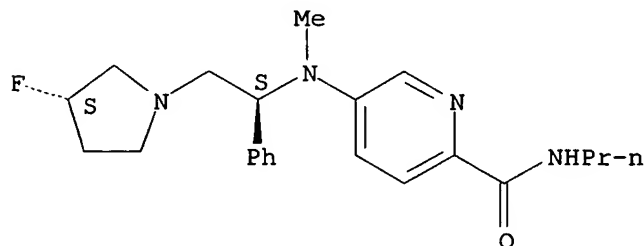
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (9CI)  
MF C22 H29 F N4 O . C4 H4 O4

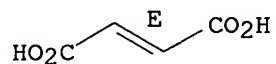
CM 1

Absolute stereochemistry.



CM 2

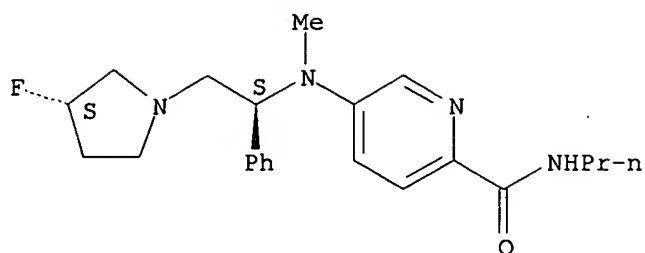
Double bond geometry as shown.



L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI)  
MF C22 H29 F N4 O  
CI COM

Absolute stereochemistry.



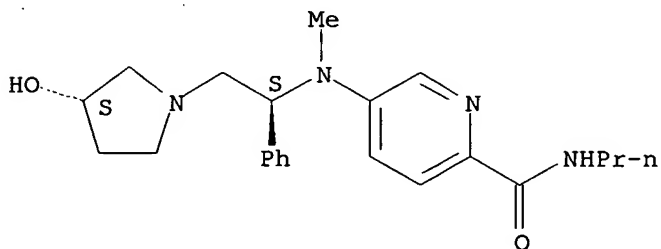


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI)  
 MF C22 H30 N4 O2 . C4 H4 O4

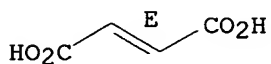
CM 1

Absolute stereochemistry.



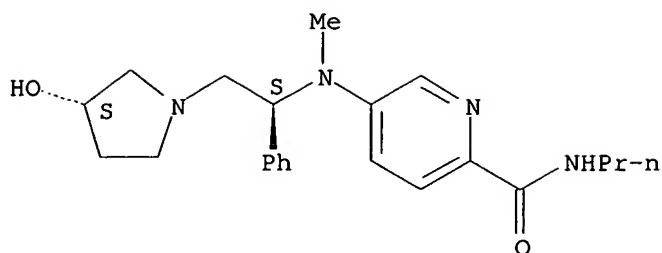
CM 2

Double bond geometry as shown.



L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI)  
 MF C22 H30 N4 O2  
 CI COM

Absolute stereochemistry.

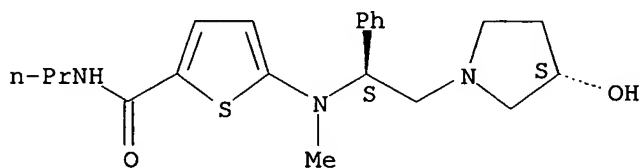


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Thiophenecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI)  
 MF C21 H29 N3 O2 S . C4 H4 O4

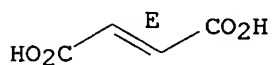
CM 1

Absolute stereochemistry.



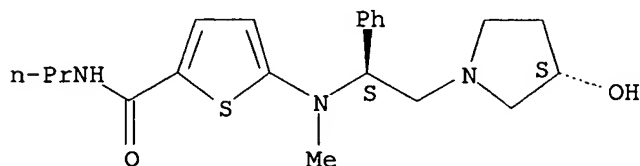
CM 2

Double bond geometry as shown.



L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Thiophenecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI)  
 MF C21 H29 N3 O2 S  
 CI COM

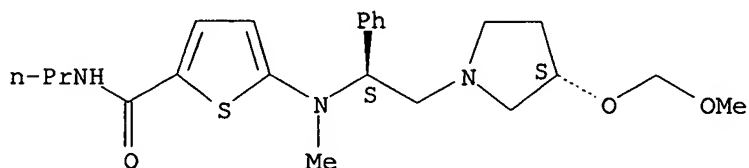
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Thiophenecarboxamide, 5-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI)  
 MF C23 H33 N3 O3 S

Absolute stereochemistry.

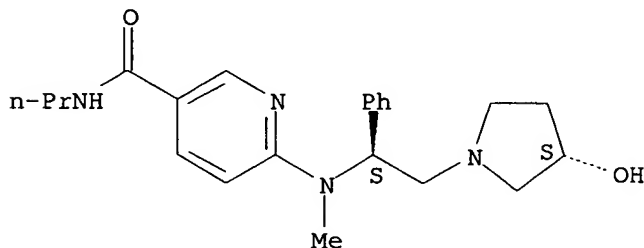


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 3-Pyridinecarboxamide, 6-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI)  
 MF C22 H30 N4 O2 . C4 H4 O4

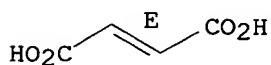
CM 1

Absolute stereochemistry.



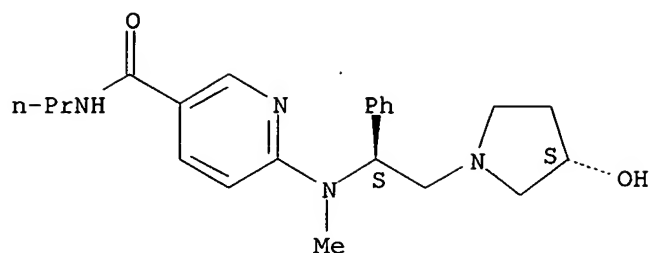
CM 2

Double bond geometry as shown.



L3 10 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 3-Pyridinecarboxamide, 6-[[[2-(3-hydroxy-1-pyrrolidinyl)-1-phenylethyl]methylamino]-N-propyl-, [S-(R\*,R\*)]- (9CI)  
 MF C22 H30 N4 O2  
 CI COM

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

161.76

161.97

FILE 'CAPLUS' ENTERED AT 18:25:20 ON 21 JAN 2005

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 21 Jan 2005 VOL 142 ISS 5

FILE LAST UPDATED: 20 Jan 2005 (20050120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3

L4 2 L3

=> d L4 ibib abs hitstr 1-2

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:178439 CAPLUS

DOCUMENT NUMBER: 134:222619

TITLE: Preparation of pyrrolidinyl- and pyrrolinylethylarylamines as kappa opioid receptor agonists

INVENTOR(S): Ito, Fumitaka; Kondo, Hiroshi

PATENT ASSIGNEE(S): Pfizer, Inc., USA

SOURCE: U.S., 39 pp., Cont.-in-part of Appl. No.

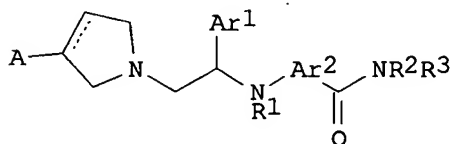
PCT/IB96/00957.

CODEN: USXXAM

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6201007	B1	20010313	US 1999-254805	19990312
WO 9812177	A1	19980326	WO 1997-IB1021	19970821
W: AU, BG, BR, CA, CN, CZ, HU, IL, IS, JP, KR, LK, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
JP 2001316344	A2	20011113	JP 2001-92342	19970821
US 2001008890	A1	20010719	US 2001-770515	20010126
US 6310061	B2	20011030		
US 2001009921	A1	20010726	US 2001-770513	20010126
US 6313302	B2	20011106		
US 2001011091	A1	20010802	US 2001-770514	20010126
US 6294569	B2	20010925		
US 2001014683	A1	20010816	US 2001-771029	20010126
US 6307061	B2	20011023		
US 2001020024	A1	20010906	US 2001-771030	20010126
US 6294557	B2	20010925		
US 6303602	B1	20011016	US 2001-770512	20010126
PRIORITY APPLN. INFO.:			WO 1996-IB957	A2 19960918
			WO 1997-IB1021	W 19970821
			JP 1998-514433	A3 19970821
			US 1999-254805	A3 19990312

OTHER SOURCE(S): MARPAT 134:222619  
 GI



AB Title compds. [I; A = H, halo, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, O, OY, null; Y = protecting group; broken line = optional double bond; Ar1 = (substituted) Ph; Ar2 = (substituted) Ph, naphththyl, pyridyl, thienyl, furyl, pyrrolyl, pyrimidinyl; R1 = H, OH, alkyl, alkoxy, OY; and R2, R3 = (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, alkoxy, Ph, etc.; R2R3N = (substituted) pyrrolidinyl, piperidinyl, morpholinyl], were prepared as  $\kappa$  agonists (no data). Thus, a mixture of 2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethanol, 2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-2-(R)-phenylethanol (preparation given), and Et3N in CH2Cl2 was treated with MeSO2Cl at 0° followed by 5,5 h stirring at room temperature to give a residue which was refluxed 1.5 h with Me 4-methylaminobenzoate in EtOH to give 62.5% Me 4-[N-[2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethyl]-N-methylamino]benzoate. This was saponified with NaOH in MeOH (quant.) and the acid was stirred with PrNH2 and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride in CH2Cl2 to give 72% Me 4-[N-[2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethyl]-N-methylamino]-N'-propylbenzamide.

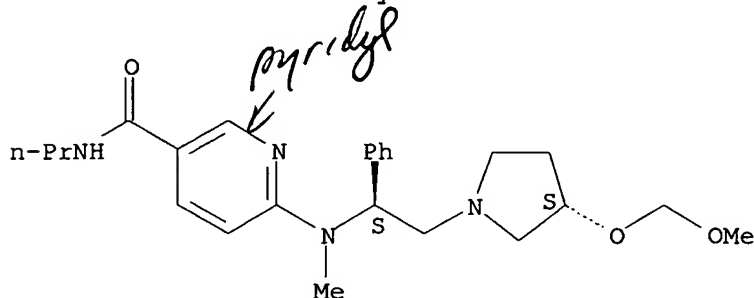
IT 204971-73-3P 204971-75-5P 204971-86-8P  
 204971-87-9P 204972-51-0P 204972-52-1P  
 204972-62-3P 204972-63-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of pyrrolidiny- and pyrrolinylethylarylamines as kappa opioid receptor agonists)

RN 204971-73-3 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-75-5 CAPLUS

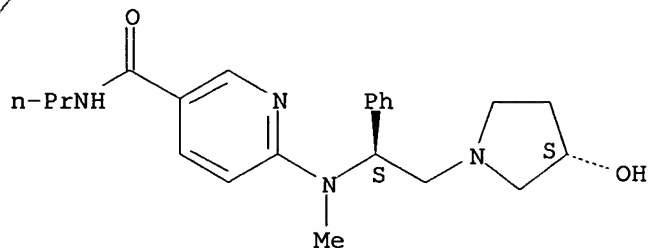
CN 3-Pyridinecarboxamide, 6-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI)  
(CA INDEX NAME)

CM 1

CRN 204971-74-4

CMF C22-H30-N4-O2

Absolute stereochemistry.

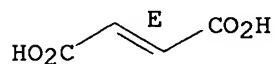


CM 2

CRN 110-17-8

CMF C4 H4 O4

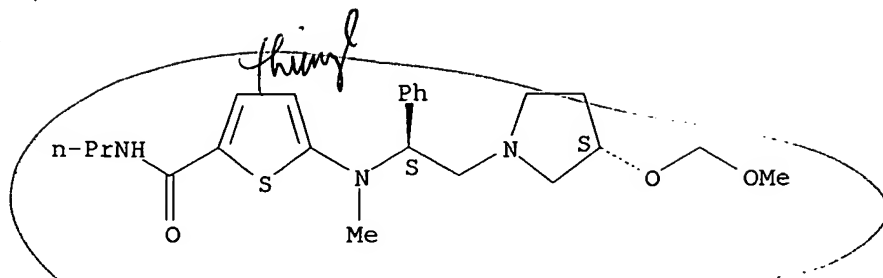
Double bond geometry as shown.



RN 204971-86-8 CAPLUS

CN 2-Thiophenecarboxamide, 5-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

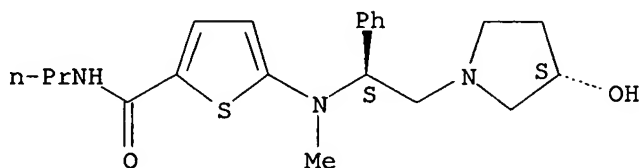
Absolute stereochemistry.



RN 204971-87-9 CAPLUS

CN 2-Thiophenecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

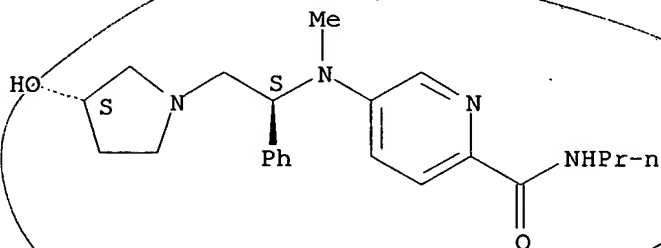
Absolute stereochemistry.



RN 204972-51-0 CAPLUS

CN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-52-1 CAPLUS

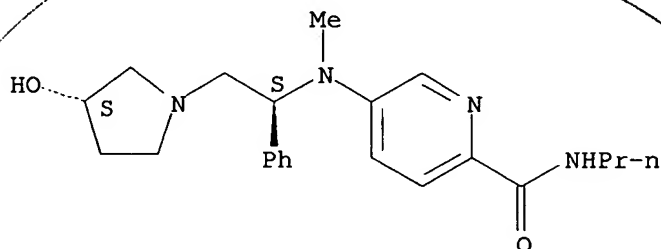
CN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204972-51-0

CMF C22 H30 N4 O2

Absolute stereochemistry.

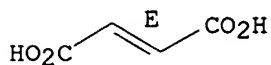


CM 2

CRN 110-17-8

CMF C4 H4 O4

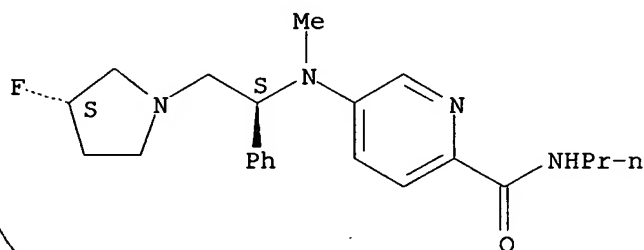
Double bond geometry as shown.



RN 204972-62-3 CAPLUS

CN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-63-4 CAPLUS

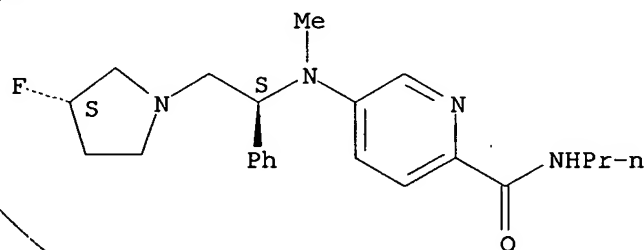
CN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

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CRN 204972-62-3

CMF C22 H29 F N4 O

Absolute stereochemistry.

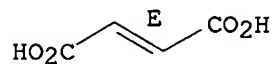


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.





REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:199673 CAPLUS

DOCUMENT NUMBER: 128:243949

TITLE: Preparation of pyrrolidinyl- and pyrrolinylethylamines as kappa agonists.

INVENTOR(S): Ito, Fumitaka; Kondo, Hiroshi

PATENT ASSIGNEE(S): Pfizer Inc., USA; Pfizer Pharmaceuticals Inc.

SOURCE: PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

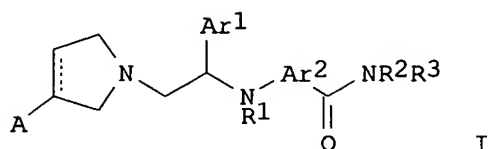
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9812177	A1	19980326	WO 1997-IB1021	19970821
W: AU, BG, BR, CA, CN, CZ, HU, IL, IS, JP, KR, LK, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
TW 432047	B	20010501	TW 1997-86111948	19970820
AU 9737812	A1	19980414	AU 1997-37812	19970821
AU 719895	B2	20000518		
EP 934264	A1	19990811	EP 1997-934676	19970821
EP 934264	B1	20030910		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LV, FI, RO				
BR 9711506	A	19990824	BR 1997-11506	19970821
CN 1237962	A	19991208	CN 1997-199817	19970821
JP 2000516634	T2	20001212	JP 1998-514433	19970821
JP 3195368	B2	20010806		
JP 2001316344	A2	20011113	JP 2001-92342	19970821
AT 249433	E	20030915	AT 1997-934676	19970821
CA 2266006	C	20031104	CA 1997-2266006	19970821
CA 2266006	AA	19980326		
PT 934264	T	20040130	PT 1997-934676	19970821
ES 2205248	T3	20040501	ES 1997-934676	19970821
AP 1016	A	20011008	AP 1997-1082	19970911
W: BW, GM, GH, KE, LS, MW, SD, SZ, UG, ZM, ZW				
ZA 9708358	A	19990317	ZA 1997-8358	19970917
BG 64194	B1	20040430	BG 1999-103239	19990311
US 6201007	B1	20010313	US 1999-254805	19990312
NO 9901294	A	19990317	NO 1999-1294	19990317
KR 2000036225	A	20000626	KR 1999-702287	19990317
US 2001008890	A1	20010719	US 2001-770515	20010126
US 6310061	B2	20011030		
US 2001009921	A1	20010726	US 2001-770513	20010126
US 6313302	B2	20011106		
US 2001011091	A1	20010802	US 2001-770514	20010126
US 6294569	B2	20010925		
US 2001014683	A1	20010816	US 2001-771029	20010126
US 6307061	B2	20011023		
US 2001020024	A1	20010906	US 2001-771030	20010126
US 6294557	B2	20010925		
US 6303602	B1	20011016	US 2001-770512	20010126
PRIORITY APPLN. INFO.:			WO 1996-IB957	A 19960918
			JP 1998-514433	A3 19970821
			WO 1997-IB1021	W 19970821

OTHER SOURCE(S):  
GI

MARPAT 128:243949



AB Title compds. [I; A = null, H, halo, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, etc.; dotted line = optional double bond; Ar1 = (substituted) Ph; Ar2 = (substituted) Ph, naphthyl, pyridyl, thienyl, furyl, pyrrolyl, pyrimidinyl; R1 = H, OH, alkyl, alkoxy, etc.; R2, R3 = H, OH, (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, alkoxy, Ph, phenylalkyl, etc.; R2R3N = (substituted) pyrrolidinyl, piperidinyl, morpholinyl], were prepared Thus, 2-[3(S)-methoxymethoxypyrrolidin-1-yl]-1(RS)-phenylethanol (preparation given) and Et3N in CH2Cl2 were treated with MeSO2Cl at 0° to give a residue which was refluxed with Me 4-methylaminobenzoate in EtOH to give 62.5% Me 4-[N-[2-[3(S)-methoxymethoxypyrrolidin-1-yl]-1(S)-phenylethyl]-N-methylamino]benzoate. This was saponified with 4N NaOH in MeOH (100%) and the resulting acid was stirred with PrNH2 and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride in CH2Cl2 to give 72% 4-[N-[2-[3(S)-methoxymethoxypyrrolidin-1-yl]-1(S)-phenylethyl]-N-methylamino]-N'-propylbenzamide. Some I inhibited acute pain in rats with ED50 <10 mg/kg orally.

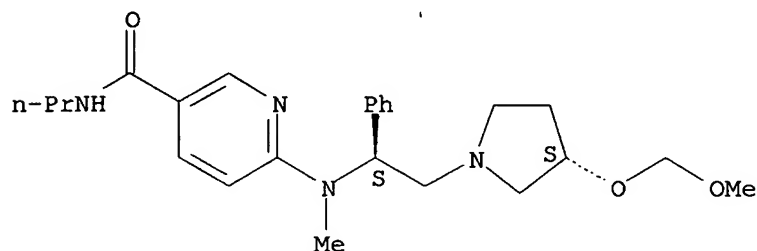
IT 204971-73-3P 204971-74-4P 204971-75-5P  
204971-86-8P 204971-87-9P 204971-88-0P  
204972-51-0P 204972-52-1P 204972-62-3P  
204972-63-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of pyrrolidinyl- and pyrrolinylethylamines as kappa agonists)

RN 204971-73-3 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl]- (9CI) (CA INDEX NAME)

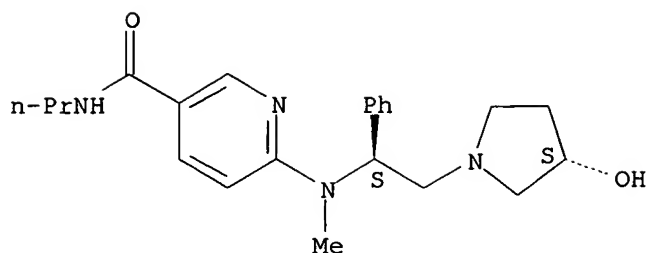
Absolute stereochemistry.



RN 204971-74-4 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[2-(3-hydroxy-1-pyrrolidinyl)-1-phenylethyl]methylamino]-N-propyl]-, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

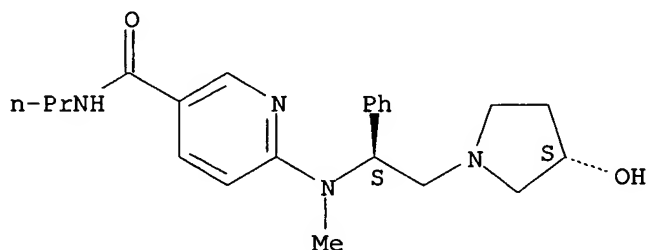


RN 204971-75-5 CAPLUS  
 CN 3-Pyridinecarboxamide, 6-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI)  
 (CA INDEX NAME)

CM 1

CRN 204971-74-4  
 CMF C22 H30 N4 O2

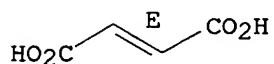
Absolute stereochemistry.



CM 2

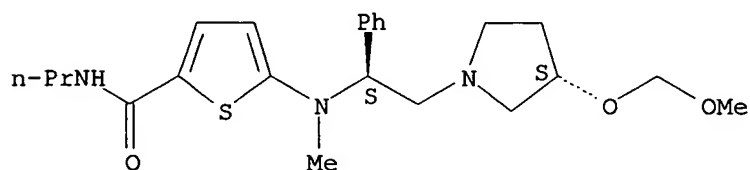
CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



RN 204971-86-8 CAPLUS  
 CN 2-Thiophenecarboxamide, 5-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

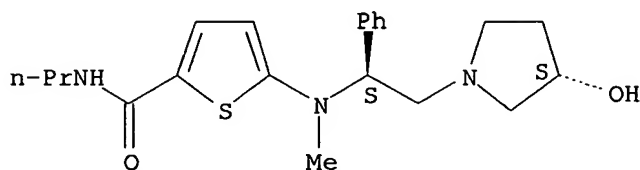
Absolute stereochemistry.



RN 204971-87-9 CAPLUS  
 CN 2-Thiophenecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-

phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-88-0 CAPLUS

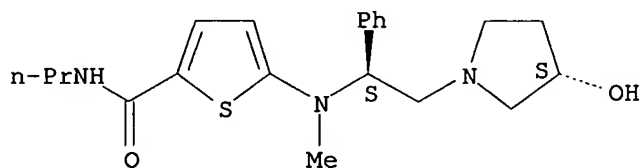
CN 2-Thiophenecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI)  
(CA INDEX NAME)

CM 1

CRN 204971-87-9

CMF C21 H29 N3 O2 S

Absolute stereochemistry.

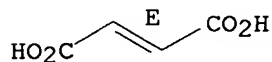


CM 2

CRN 110-17-8

CMF C4 H4 O4

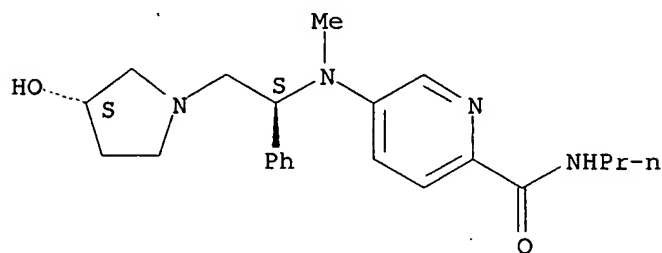
Double bond geometry as shown.



RN 204972-51-0 CAPLUS

CN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-52-1 CAPLUS

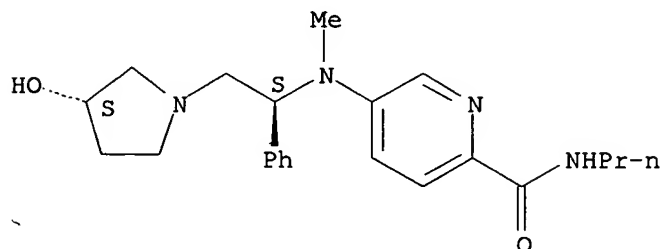
CN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-

phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI)  
(CA INDEX NAME)

CM 1

CRN 204972-51-0  
CMF C22 H30 N4 O2

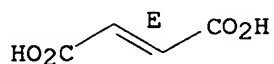
Absolute stereochemistry.



CM 2

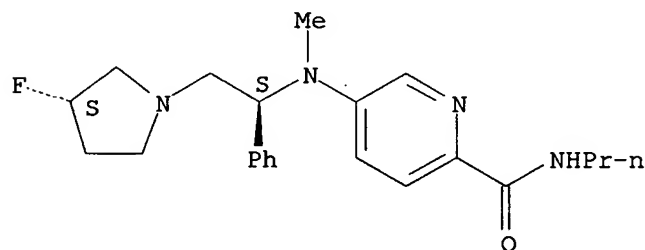
CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.



RN 204972-62-3 CAPLUS  
CN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-63-4 CAPLUS  
CN 2-Pyridinecarboxamide, 5-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 204972-62-3  
CMF C22 H29 F N4 O

Absolute stereochemistry.

Connecting via Winsock to STN

106991066

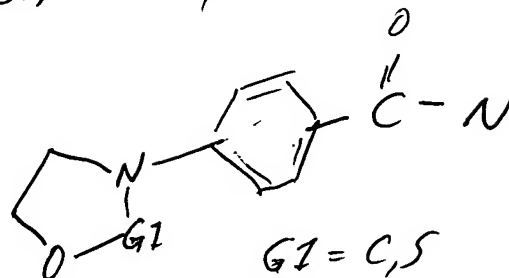
1/21/05

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LOGINID:SSSPTAAJP1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2



\* \* \* \* \* Welcome to STN International \* \* \* \* \*

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NEWS 2 "Ask CAS" for self-help around the clock  
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NEWS 5 NOV 30 PHAR reloaded with additional data  
NEWS 6 DEC 01 LISA now available on STN  
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NEWS 8 DEC 15 MEDLINE update schedule for December 2004  
NEWS 9 DEC 17 ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 10 DEC 17 COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 11 DEC 17 SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 12 DEC 17 CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 13 DEC 17 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB  
NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN  
NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED  
NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and February 2005  
NEWS 17 JAN 11 CA/CAPLUS - Expanded patent coverage to include Russia (Federal Institute of Industrial Property)  
  
NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Organic Letter  
Chosh of L.  
June 26  
2003  
compd 23  
p. 2209  
Table 2

(compd VI)  
and (VII)

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COST IN U.S. DOLLARS

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TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

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STRUCTURE FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

DICTIONARY FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

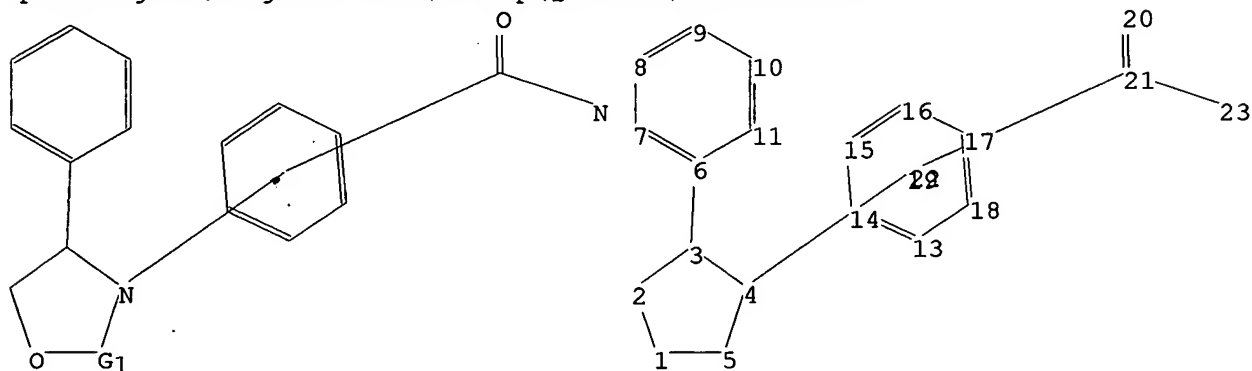
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10699106d.str



chain nodes :

20 21 23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 13 14 15 16 17 18

chain bonds :

3-6 20-21 21-23

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 13-14 13-18 14-15  
15-16 16-17 17-18

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5 20-21 21-23

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11 13-14 13-18 14-15 15-16 16-17 17-18

G1:C,S

Match level :

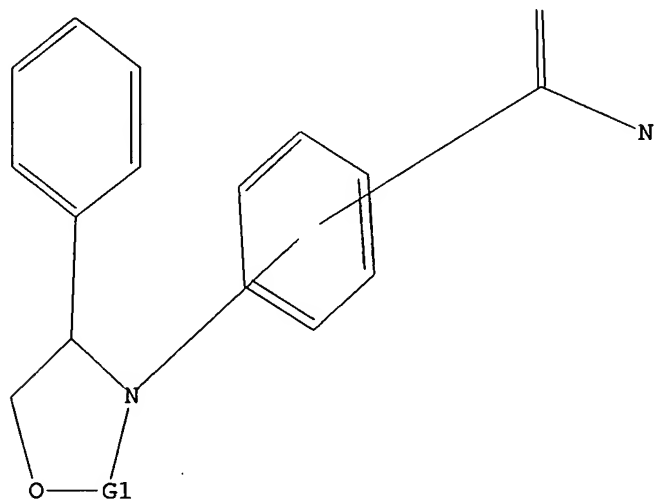
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11:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS  
21:CLASS 22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 C,S

Structure attributes must be viewed using STN Express query preparation.

=> s L1

SAMPLE SEARCH INITIATED 19:17:47 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1347 TO ITERATE

74.2% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 24739 TO 29141

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 19:17:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 27114 TO ITERATE

100.0% PROCESSED 27114 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01



L3 4 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

161.33

161.54

FILE 'CAPLUS' ENTERED AT 19:18:07 ON 21 JAN 2005

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FILE COVERS 1907 - 21 Jan 2005 VOL 142 ISS 5

FILE LAST UPDATED: 20 Jan 2005 (20050120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.45

161.99

FILE 'REGISTRY' ENTERED AT 19:18:12 ON 21 JAN 2005

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STRUCTURE FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

DICTIONARY FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d L3 1-4 all

L3 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN

RN 686347-75-1 REGISTRY

ED Entered STN: 27 May 2004

CN Benzamide, 4-(2,2-dioxido-4-phenyl-1,2,3-oxathiazolidin-3-yl)-N-propyl-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-(2,2-Dioxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide

FS 3D CONCORD

MF C18 H20 N2 O4 S

SR CA

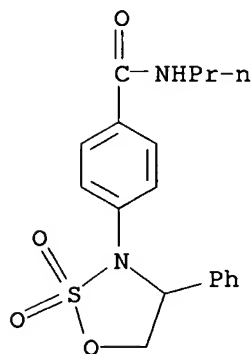
LC STN Files: CA, CAPLUS, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C2NOS	NSOC2	5	C2NOS	16.272.1	1
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	16.8	pH 1	(1) ACD
Bioconc. Factor (BCF)	16.8	pH 4	(1) ACD
Bioconc. Factor (BCF)	16.8	pH 7	(1) ACD
Bioconc. Factor (BCF)	16.8	pH 8	(1) ACD
Bioconc. Factor (BCF)	16.8	pH 10	(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	262	pH 1	(1) ACD
Koc (KOC)	262	pH 4	(1) ACD
Koc (KOC)	262	pH 7	(1) ACD
Koc (KOC)	262	pH 8	(1) ACD
Koc (KOC)	262	pH 10	(1) ACD
logD (LOGD)	1.91	pH 1	(1) ACD
logD (LOGD)	1.91	pH 4	(1) ACD
logD (LOGD)	1.91	pH 7	(1) ACD

logD (LOGD)	1.91	pH 8	(1) ACD
logD (LOGD)	1.91	pH 10	(1) ACD
logP (LOGP)	1.915+/-0.687		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	360.43		(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

AN 140:391196 CA  
 TI Process for the preparation of pyrrolidinyl ethylamine compounds via a  
 copper-mediated aryl amination  
 IN Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel  
 PA Pfizer Products Inc., USA  
 SO PCT Int. Appl., 34 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D  
 ICS C07D291-04; C07D207-12  
 CC 27-10 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 45

*our app*

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004039785	A1	20040513	WO 2003-IB4676	20031022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2004152896 A1 20040805 US 2003-699106 20031031 PRAI US 2002-423328P 20021101 GI				

*our apps*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention provides a new process for the preparation of the well-known  
 kappa agonists I via a copper salt-catalyzed amination of an oxazolidinone  
 II with an aryl halide III in the presence of an amino ligand and a base  
 [wherein A = H, OH and derivs., fluoro/alkyl, etc.; Ar1 = (un)substituted  
 phenyl; Ar2 = (un)substituted Ph, naphthyl, pyridinyl, thiophenyl, furyl,  
 pyrrolyl, pyrimidinyl; R1 = alkyl, benzyl, with its Ph part optionally  
 substituted; R2, R3 = independently H, (un)substituted alkyl, or R2R3N =

(un)substituted pyrrolidine, piperidine, morpholine; X = Cl, Br, I]. The advantages of the aryl amination include high yields, mild, efficient, cost-effective and robust process. For example, aryl amination of S-(+)-4-phenyloxazolidin-2-one with 4-bromo-N-propylbenzamide in the presence of CuI/K<sub>2</sub>CO<sub>3</sub> gave the intermediate IV, used in the synthesis of pyrrolidinyl ethylamine V.

ST pyrrolidinyl ethylamine prepn copper aryl amination

IT Amination  
(aryl; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT Amination catalysts  
(process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT Amines, preparation  
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(products; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT Aryl halides  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 686347-77-3P, Benzoic acid 1-[2-[methyl[4-(propylcarbamoyl)phenyl]amino]-2-phenylethyl]pyrrolidin-3-yl ester  
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(amine product; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 497-19-8, Sodium carbonate, uses 534-17-8, Cesium carbonate 584-08-7, Potassium carbonate  
RL: NUU (Other use, unclassified); USES (Uses)  
(base; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 7681-65-4, Copper iodide (CuI) 7758-89-6, Copper chloride (CuCl) 7787-70-4, Copper bromide (CuBr)  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 686347-72-8P, 4-(2-Oxo-4-phenyloxazolidin-3-yl)-N-propylbenzamide  
686347-73-9P, 4-[(2-Hydroxy-1-phenylethyl)amino]-N-propylbenzamide  
686347-74-0P, 4-(2-Oxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide 686347-75-1P, 4-(2,2-Dioxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide 686347-76-2P, Benzoic acid 1-[2-phenyl-2-[[4-(propylcarbamoyl)phenyl]amino]ethyl]pyrrolidin-3-yl ester  
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 694-83-7, 1,2-Diaminocyclohexane  
RL: CAT (Catalyst use); USES (Uses)  
(ligand; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 99395-88-7, (S)-(+)-4-Phenyloxazolidin-2-one 99855-14-8, Benzoic acid pyrrolidin-3-yl ester hydrochloride 223557-19-5, 4-Bromo-N-propylbenzamide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

L3 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN

RN 686347-74-0 REGISTRY

ED Entered STN: 27 May 2004

CN Benzamide, 4-(2-oxido-4-phenyl-1,2,3-oxathiazolidin-3-yl)-N-propyl- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN 4-(2-Oxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide

FS 3D CONCORD

MF C18 H20 N2 O3 S

SR CA

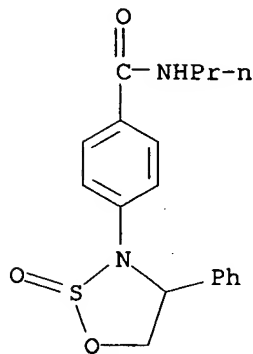
LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Caplus document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C2NOS	NSOC2	5	C2NOS	16.272.1	1
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	9.71	pH 1	(1) ACD
Bioconc. Factor (BCF)	9.72	pH 4	(1) ACD
Bioconc. Factor (BCF)	9.72	pH 7	(1) ACD
Bioconc. Factor (BCF)	9.72	pH 8	(1) ACD
Bioconc. Factor (BCF)	9.72	pH 10	(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	177	pH 1	(1) ACD
Koc (KOC)	177	pH 4	(1) ACD
Koc (KOC)	177	pH 7	(1) ACD
Koc (KOC)	177	pH 8	(1) ACD
Koc (KOC)	177	pH 10	(1) ACD
logD (LOGD)	1.60	pH 1	(1) ACD
logD (LOGD)	1.60	pH 4	(1) ACD
logD (LOGD)	1.60	pH 7	(1) ACD

logD (LOGD)	1.60	pH 8	(1) ACD
logD (LOGD)	1.60	pH 10	(1) ACD
logP (LOGP)	1.603+/-0.669		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	344.43		(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

AN 140:391196 CA  
 TI Process for the preparation of pyrrolidinyl ethylamine compounds via a  
 copper-mediated aryl amination  
 IN Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel  
 PA Pfizer Products Inc., USA  
 SO PCT Int. Appl., 34 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D  
 ICS C07D291-04; C07D207-12  
 CC 27-10 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 45

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004039785	A1	20040513	WO 2003-IB4676	20031022
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2004152896	A1	20040805	US 2003-699106	20031031
PRAI	US 2002-423328P		20021101		
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention provides a new process for the preparation of the well-known kappa agonists I via a copper salt-catalyzed amination of an oxazolidinone II with an aryl halide III in the presence of an amino ligand and a base [wherein A = H, OH and derivs., fluoro/alkyl, etc.; Ar1 = (un)substituted phenyl; Ar2 = (un)substituted Ph, naphthyl, pyridinyl, thiophenyl, furyl, pyrrolyl, pyrimidinyl; R1 = alkyl, benzyl, with its Ph part optionally substituted; R2, R3 = independently H, (un)substituted alkyl, or R2R3N =

(un)substituted pyrrolidine, piperidine, morpholine; X = Cl, Br, I]. The advantages of the aryl amination include high yields, mild, efficient, cost-effective and robust process. For example, aryl amination of S-(+)-4-phenyloxazolidin-2-one with 4-bromo-N-propylbenzamide in the presence of CuI/K<sub>2</sub>CO<sub>3</sub> gave the intermediate IV, used in the synthesis of pyrrolidinyl ethylamine V.

ST pyrrolidinyl ethylamine prepn copper aryl amination

IT Amination  
(aryl; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT Amination catalysts  
(process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT Amines, preparation  
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(products; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT Aryl halides  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 686347-77-3P, Benzoic acid 1-[2-[methyl[4-(propylcarbamoyl)phenyl]amino]-2-phenylethyl]pyrrolidin-3-yl ester  
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(amine product; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 497-19-8, Sodium carbonate, uses 534-17-8, Cesium carbonate 584-08-7, Potassium carbonate  
RL: NUU (Other use, unclassified); USES (Uses)  
(base; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 7681-65-4, Copper iodide (CuI) 7758-89-6, Copper chloride (CuCl) 7787-70-4, Copper bromide (CuBr)  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 686347-72-8P, 4-(2-Oxo-4-phenyloxazolidin-3-yl)-N-propylbenzamide  
686347-73-9P, 4-[(2-Hydroxy-1-phenylethyl)amino]-N-propylbenzamide  
686347-74-0P, 4-(2-Oxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide 686347-75-1P, 4-(2,2-Dioxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide 686347-76-2P, Benzoic acid 1-[2-phenyl-2-[[4-(propylcarbamoyl)phenyl]amino]ethyl]pyrrolidin-3-yl ester  
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 694-83-7, 1,2-Diaminocyclohexane  
RL: CAT (Catalyst use); USES (Uses)  
(ligand; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 99395-88-7, (S)-(+)-4-Phenyloxazolidin-2-one 99855-14-8, Benzoic acid pyrrolidin-3-yl ester hydrochloride 223557-19-5, 4-Bromo-N-propylbenzamide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

L3 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN

RN 686347-72-8 REGISTRY

ED Entered STN: 27 May 2004

CN Benzamide, 4-(2-oxo-4-phenyl-3-oxazolidinyl)-N-propyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-[4-[(Propylamino)carbonyl]phenyl]-4-phenyloxazolidin-2-one

CN 4-(2-Oxo-4-phenyloxazolidin-3-yl)-N-propylbenzamide

FS 3D CONCORD

MF C19 H20 N2 O3

SR CA

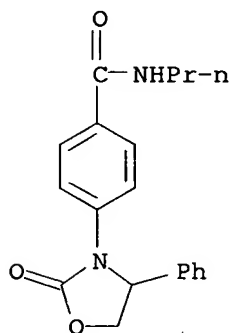
LC STN Files: CA, CAPLUS, USPATFULL

DT.CA CAPLUS document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3NO	NCOC2	5	C3NO	16.239.1	1
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	30.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	30.1	pH 4	(1) ACD
Bioconc. Factor (BCF)	30.1	pH 7	(1) ACD
Bioconc. Factor (BCF)	30.1	pH 8	(1) ACD
Bioconc. Factor (BCF)	30.1	pH 10	(1) ACD
Boiling Point (BP)	528.4+/-49.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	80.32+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	273.3+/-53.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	397	pH 1	(1) ACD
Koc (KOC)	398	pH 4	(1) ACD
Koc (KOC)	398	pH 7	(1) ACD
Koc (KOC)	398	pH 8	(1) ACD
Koc (KOC)	398	pH 10	(1) ACD



logD (LOGD)	2.25	pH 1	(1) ACD
logD (LOGD)	2.25	pH 4	(1) ACD
logD (LOGD)	2.25	pH 7	(1) ACD
logD (LOGD)	2.25	pH 8	(1) ACD
logD (LOGD)	2.25	pH 10	(1) ACD
logP (LOGP)	2.248+/-0.644		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	324.37		(1) ACD
Vapor Pressure (VP)	2.99E-11 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

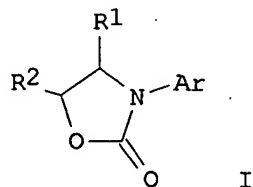
See HELP PROPERTIES for information about property data sources in REGISTRY.  
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

AN 140:406800 CA  
TI Methods for preparing N-aryl oxazolidinones via a copper catalyzed cross  
coupling reaction  
IN Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel  
PA Pfizer Products Inc., USA  
SO PCT Int. Appl., 28 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
IC ICM C07D263-22  
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))  
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004039788	A1	20040513	WO 2003-IB4708	20031022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2004122226 A1 20040624 US 2003-645779 20030821 PRAI US 2002-423328P 20021101 US 2003-645779 20030821				

GI



*us 20040122226 A1 (6/24/03)*

AB Methods for the preparation of N-aryl oxazolidinones (shown as I; variables defined below; e.g. (R)-4-ethyl-3-(4-trifluoromethylphenyl)oxazolidin-2-one (II)) via a Cu catalyzed cross coupling reaction are disclosed. These compds. are intermediates useful in the preparation of cholesteryl ester transfer protein inhibitors. Preferred catalyst ligands are MeNHCH<sub>2</sub>CH<sub>2</sub>NHMe and 1,2-diaminocyclohexane. For example, II was prepared by charging K<sub>2</sub>CO<sub>3</sub> (87 mmol) and CuI (4.4 mmol) to a flask under N<sub>2</sub> and adding (R)-4-ethyloxazolidin-2-one (43.5 mmol) and 1-bromo-4-trifluoromethylbenzene (42.8 mmol) each diluted in 20 mL dioxane to the flask followed by 1,2-diaminocyclohexane (4.4 mmol); the bright blue mixture was heated to 110° and held for 22 h; workup gave 86 % product. Further examples describe the conversion of II to (R)-2-(4-trifluoromethylphenylamino)butan-1-ol (97 %), (R)-4-ethyl-3-(4-trifluoromethylphenyl)-[1,2,3]oxathiazolidine 2-oxide (81 %) and finally (R)-3-(4-trifluoromethylphenylamino)pentanenitrile (81 %). Six addnl. examples of preparation of I are included. For I: R<sub>1</sub> is a partially saturated, fully saturated or fully unsatd. (C1-C4) straight or branched C chain wherein the carbons, other than the connecting C, may optionally be replaced with one heteroatom = O, S and N wherein said C atoms are optionally mono, di- or trisubstituted independently with halo, said C is optionally monosubstituted with oxo or hydroxy, said S is optionally mono- or disubstituted with oxo, said N is optionally mono- or disubstituted with oxo; or said R<sub>1</sub> is a partially saturated, fully saturated or fully unsatd. 3-5-membered ring optionally having one heteroatom = O, S and N; wherein said R<sub>1</sub> ring is optionally mono, di- or trisubstituted independently with halo, (C1-C6)alkoxy, nitro, (C1-C4)alkyloxycarbonyl. R<sub>2</sub> is H, C1-C4 alkyl, C3-C6 cycloalkyl, C2-C6 alkenyl, C2-C6 alkynyl, C1-C4 alkoxy, C1-C4 alkoxy-C1-C4 alkyl; Ph (un)substituted with C1-C6 alkoxy or OY wherein Y is a hydroxy protecting group, halogen, C1-C4 alkyl, C2-C6 alkenyl, C2-C6 alkynyl, C1-C4 alkoxy, C1-C4 alkoxy-C1-C4 alkyl, trifluoromethyl, nitro, carbo-C1-C4 alkoxy, C1-C4 alkoxy-carbonyl, carbonyl, or cyano; or benzyl with the Ph moiety of the benzyl (un)substituted with C1-C6 alkoxy or OY wherein Y is a hydroxy protecting group, halogen, C1-C4 alkyl, C2-C6 alkenyl, C2-C6 alkynyl, C1-C4 alkoxy, C1-C4 alkoxy-C1-C4 alkyl, trifluoromethyl, amido, nitro, carbo-C1-C4 alkoxy, C1-C4 alkoxy-carbonyl, carbonyl or cyano; wherein Ar is an aromatic hydrocarbon or heteroarom. moiety Ph, naphthyl, pyridyl, thiophenyl, furanyl, pyrrolyl and pyrimidyl, imidazolyl, oxazolyl, thiazolyl, triazolyl, pyrazolyl, pyrazinyl, pyridazinyl each of which may be (un)substituted by ≥1, preferably 1-2, substituents = halo, hydroxy, C1-C4 alkyl, C2-C6 alkenyl, C2-C6 alkynyl, C1-C4 alkoxy, C1-C4 alkoxy-C1-C4 alkyl, CF<sub>3</sub>, amino, amido, imines, nitro, carbo-C1-C4 alkoxy, C1-C4 alkoxy-carbonyl, carbonyls (ketones and aldehydes), cyano.

ST Arylation  
IT Arylation  
Arylation catalysts  
Cross-coupling reaction  
Cross-coupling reaction catalysts  
(methods for preparing N-aryl oxazolidinones via copper catalyzed cross coupling reaction)

IT 19319-86-9, Dibromo(o-phenanthroline)copper  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst comparison; methods for preparing N-aryl oxazolidinones via copper catalyzed cross coupling reaction)

IT 66-71-7, o-Phenanthroline 107-15-3, Ethylenediamine, uses 107-21-1, Ethylene glycol, uses 109-83-1, 2-(Methylamino)ethanol 110-70-3, N,N'-Dimethylethylenediamine 366-18-7, 2,2'-Bipyridine 1121-22-8, trans-1,2-Diaminocyclohexane 67579-81-1, trans-1,2-Bis(methylamino)cyclohexane  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst ligand comparison; methods for preparing N-aryl oxazolidinones via copper catalyzed cross coupling reaction)

IT 108-00-9, N,N-Dimethylethylenediamine 694-83-7, 1,2-Diaminocyclohexane  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst ligand; methods for preparing N-aryl oxazolidinones via copper catalyzed cross coupling reaction)

IT 99-90-1, 4'-Bromoacetophenone 106-37-6, 1,4-Dibromobenzene 108-86-1, Phenyl bromide, reactions 352-34-1, 4-Fluorophenyl iodide 402-43-7, 4-(Trifluoromethyl)phenyl bromide 455-13-0, 4-(Trifluoromethyl)phenyl iodide 591-50-4, Phenyl iodide 623-00-7, 4-Cyanophenyl bromide 5856-63-3, (R)-2-Amino-1-butanol 7480-32-2, 4-Phenyloxazolidin-2-one 16112-60-0, 4-Ethyloxazolidin-2-one 17016-83-0, (S)-4-Isopropylloxazolidin-2-one 90319-52-1, (R)-4-Phenyloxazolidin-2-one 99395-88-7, (S)-4-Phenyloxazolidin-2-one 223557-19-5, 4-Bromo-N-propylbenzamide 330555-60-7, (S)-5-[(Trityloxy)methyl]oxazolidin-2-one  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (methods for preparing N-aryl oxazolidinones via copper catalyzed cross coupling reaction)

IT 98974-04-0P, (R)-4-Ethyloxazolidin-2-one 688789-23-3P, (R)-4-Ethyl-3-(4-trifluoromethylphenyl)oxazolidin-2-one 688789-24-4P, (R)-2-(4-Trifluoromethylphenylamino)butan-1-ol 688789-25-5P, (3R)-4-Ethyl-3-(4-trifluoromethylphenyl)-[1,2,3]oxathiazolidine 2-oxide  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (methods for preparing N-aryl oxazolidinones via copper catalyzed cross coupling reaction)

IT 13606-71-8P, 3,4-Diphenyloxazolidin-2-one 474645-91-5P, (R)-3-(4-Trifluoromethylphenylamino)pentanenitrile 513068-72-9P, 3-(4-Cyanophenyl)-4-phenyloxazolidin-2-one 572923-34-3P, (S)-3,4-Diphenyloxazolidin-2-one 686347-72-8P, 3-[4-[(Propylamino)carbonyl]phenyl]-4-phenyloxazolidin-2-one 688789-20-0P, 3-[4-(Trifluoromethyl)phenyl]-4-phenyloxazolidin-2-one 688789-21-1P, 3-(4-Fluorophenyl)-4-phenyloxazolidin-2-one 688789-22-2P, 3-[4-(Trifluoromethyl)phenyl]-4-ethyloxazolidin-2-one 688789-26-6P, (S)-4-(4-Isopropyl-2-oxooxazolidin-3-yl)-N-propylbenzamide 688789-27-7P, (R)-3,4-Diphenyloxazolidin-2-one 688789-28-8P, (R)-4-(2-Oxo-4-phenyloxazolidin-3-yl)benzonitrile 688789-29-9P, (S)-3-(4-Acetylphenyl)-5-[(trityloxy)methyl]oxazolidin-2-one 688789-30-2P, (R)-3-(4-Bromophenyl)-4-phenyloxazolidin-2-one  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (methods for preparing N-aryl oxazolidinones via copper catalyzed cross coupling reaction)

## REFERENCE 2

AN 140:391196 CA  
 TI Process for the preparation of pyrrolidinyl ethylamine compounds via a copper-mediated aryl amination  
 IN Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel  
 PA Pfizer Products Inc., USA  
 SO PCT Int. Appl., 34 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D  
 ICS C07D291-04; C07D207-12  
 CC 27-10 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 45  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004039785	A1	20040513	WO 2003-IB4676	20031022
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,				

GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,  
 LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,  
 OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,  
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,  
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004152896 A1 20040805 US 2003-699106 20031031

PRAI US 2002-423328P 20021101

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

- AB The invention provides a new process for the preparation of the well-known kappa agonists I via a copper salt-catalyzed amination of an oxazolidinone II with an aryl halide III in the presence of an amino ligand and a base [wherein A = H, OH and derivs., fluoro/alkyl, etc.; Ar1 = (un)substituted phenyl; Ar2 = (un)substituted Ph, naphthyl, pyridinyl, thiophenyl, furyl, pyrrolyl, pyrimidinyl; R1 = alkyl, benzyl, with its Ph part optionally substituted; R2, R3 = independently H, (un)substituted alkyl, or R2R3N = (un)substituted pyrrolidine, piperidine, morpholine; X = Cl, Br, I]. The advantages of the aryl amination include high yields, mild, efficient, cost-effective and robust process. For example, aryl amination of S-(+)-4-phenyloxazolidin-2-one with 4-bromo-N-propylbenzamide in the presence of CuI/K2CO3 gave the intermediate IV, used in the synthesis of pyrrolidinyl ethylamine V.
- ST pyrrolidinyl ethylamine prepn copper aryl amination
- IT Amination  
 (aryl; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)
- IT Amination catalysts  
 (process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)
- IT Amines, preparation  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (products; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)
- IT Aryl halides  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (starting material; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)
- IT 686347-77-3P, Benzoic acid 1-[2-[methyl[4-(propylcarbamoyl)phenyl]amino]-2-phenylethyl]pyrrolidin-3-yl ester  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (amine product; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)
- IT 497-19-8, Sodium carbonate, uses 534-17-8, Cesium carbonate 584-08-7, Potassium carbonate  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (base; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)
- IT 7681-65-4, Copper iodide (CuI) 7758-89-6, Copper chloride (CuCl) 7787-70-4, Copper bromide (CuBr)  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)
- IT 686347-72-8P, 4-(2-Oxo-4-phenyloxazolidin-3-yl)-N-propylbenzamide

686347-73-9P, 4-[(2-Hydroxy-1-phenylethyl)amino]-N-propylbenzamide  
 686347-74-0P, 4-(2-Oxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide 686347-75-1P, 4-(2,2-Dioxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide 686347-76-2P, Benzoic acid 1-[2-phenyl-2-[[4-(propylcarbamoyl)phenyl]amino]ethyl]pyrrolidin-3-yl ester

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 694-83-7, 1,2-Diaminocyclohexane

RL: CAT (Catalyst use); USES (Uses)

(ligand; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

IT 99395-88-7, (S)-(+)-4-Phenyloxazolidin-2-one 99855-14-8, Benzoic acid pyrrolidin-3-yl ester hydrochloride 223557-19-5, 4-Bromo-N-propylbenzamide

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

L3 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN

RN 572923-17-2 REGISTRY

ED Entered STN: 25 Aug 2003

CN Benzamide, 4-[(4S)-2-oxo-4-phenyl-3-oxazolidinyl]-N-propyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H20 N2 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT

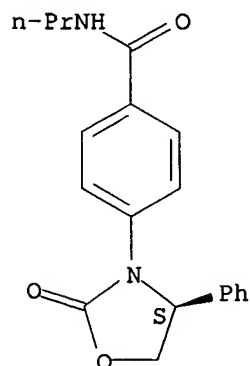
DT.CA CAPLUS document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3NO	NCOC2	5	C3NO	16.239.1	1
C6	C6	6	C6	46.150.18	2

Absolute stereochemistry.



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	30.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	30.1	pH 4	(1) ACD
Bioconc. Factor (BCF)	30.1	pH 7	(1) ACD
Bioconc. Factor (BCF)	30.1	pH 8	(1) ACD
Bioconc. Factor (BCF)	30.1	pH 10	(1) ACD
Boiling Point (BP)	528.4+/-49.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	80.32+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	273.3+/-53.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	397	pH 1	(1) ACD
Koc (KOC)	398	pH 4	(1) ACD
Koc (KOC)	398	pH 7	(1) ACD
Koc (KOC)	398	pH 8	(1) ACD
Koc (KOC)	398	pH 10	(1) ACD
logD (LOGD)	2.25	pH 1	(1) ACD
logD (LOGD)	2.25	pH 4	(1) ACD
logD (LOGD)	2.25	pH 7	(1) ACD
logD (LOGD)	2.25	pH 8	(1) ACD
logD (LOGD)	2.25	pH 10	(1) ACD
logP (LOGP)	2.248+/-0.644		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	324.37		(1) ACD
Vapor Pressure (VP)	2.99E-11 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

AN 139:149559 CA  
 TI Palladium-Catalyzed Synthesis of N-Aryloxazolidinones from Aryl Chlorides  
 AU Ghosh, Arun; Sieser, Janice E.; Riou, Maxime; Cai, Weiling; Rivera-Ruiz, Luis  
 CS Process Research and Development, Pfizer Global Research and Development, Groton, CT, 06340-8013, USA  
 SO Organic Letters (2003), 5(13), 2207-2210  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))  
 AB An efficient method for intermol. N-arylation of oxazolidinones using Pd2dba3 and various phosphine ligands in the presence of a weak base is reported. The conditions allow the use of cheaper aryl chlorides containing functionalities such as enolizable ketones, amides, etc., which would be

June 26, 2003  
 compd # 23, p 2209

have  
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incompatible with other coupling methods. The coupling reaction can be used to prepare enantiopure N-aryl  $\beta$ -amino alcs. Depending on the stereoelectronic nature of the aryl chloride, careful choice of ligand was necessary for the success of these reactions.

ST oxazolidinone arylation aryl chloride phosphine palladium catalyst;  
aryloxazolidinone prepn hydrolysis; arylaminoalkanol prepn

IT Alcohols, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(amino; palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

IT Aryl halides  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(aryl chlorides; palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

IT Chlorides, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(aryl; palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

IT Arylation  
Arylation catalysts  
(palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

IT 51364-51-3 213697-53-1 224311-51-7, 2-Di-tert-butylphosphino-1,1'-biphenyl 247940-06-3, 2-Dicyclohexylphosphino-1,1'-biphenyl  
RL: CAT (Catalyst use); USES (Uses)  
(palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

IT 98-56-6, 1-Chloro-4-trifluoromethylbenzene 99-02-5 99-91-2 100-00-5, 1-Chloro-4-nitrobenzene 104-88-1, 4-Chlorobenzaldehyde, reactions 106-43-4, 4-Chlorotoluene 108-90-7, Chlorobenzene, reactions 623-03-0, 4-Chlorobenzonitrile 623-12-1, 4-Chloroanisole 873-32-5, 2-Chlorobenzonitrile 1126-46-1, Methyl 4-chlorobenzoate 2845-89-8, 3-Chloroanisole 4042-35-7, (S)-4-Methyl-2-oxazolidinone 7461-32-7, 4-Chloro-N-propylbenzamide 13896-06-5, (S)-4-Ethyl-2-oxazolidinone 16112-59-7, 4-Methyl-2-oxazolidinone 17016-83-0, (S)-4-Isopropyl-2-oxazolidinone 99395-88-7, (+)-4-Phenyl-2-oxazolidinone 102029-44-7, (+)-4-Benzyl-2-oxazolidinone 572923-34-3 572923-35-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

IT 572922-96-4P 572922-97-5P 572922-98-6P 572922-99-7P 572923-05-8P 572923-06-9P 572923-07-0P 572923-10-5P 572923-11-6P 572923-12-7P 572923-18-3P 572923-20-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

IT 534-17-8, Cesium carbonate  
RL: RGT (Reagent); RACT (Reactant or reagent)  
(palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

IT 135285-98-2P 413190-46-2P 572923-00-3P 572923-01-4P 572923-02-5P 572923-03-6P 572923-04-7P 572923-08-1P 572923-09-2P 572923-13-8P 572923-14-9P 572923-15-0P 572923-16-1P 572923-17-2P 572923-19-4P 572923-21-8P 572923-22-9P 572923-23-0P 572923-24-1P 572923-25-2P 572923-26-3P 572923-27-4P 572923-28-5P 572923-29-6P 572923-30-9P 572923-31-0P 572923-32-1P 572923-33-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD  
(1) Arterburn, J; Org Lett 2001, V3, P1351 CAPLUS  
(2) Cacchi, S; Org Lett 2001, V3, P2539 CAPLUS

- (3) Dai, C; J Am Chem Soc 2001, V123, P2719 CAPLUS
- (4) Fox, J; J Am Chem Soc 2000, V122, P1360 CAPLUS
- (5) Genin, M; J Med Chem 1998, V41, P5144 CAPLUS
- (6) Gleave, D; Bioorg Med Chem Lett 1998, V8, P1231 CAPLUS
- (7) Gleave, D; J Org Chem 1996, V61, P6470 CAPLUS
- (8) Grushin, V; Chem Rev 1994, V94, P1047 CAPLUS
- (9) Guari, Y; Chem Eur J 2001, V7, P475 CAPLUS
- (10) Guari, Y; Tetrahedron Lett 1999, V40, P3789 CAPLUS
- (11) Halle, E; Chemother J 2002, V11, P1 CAPLUS
- (12) Harris, M; J Org Chem 1999, V64, P6019 CAPLUS
- (13) Hartwig, J; Angew Chem, Int Ed 1998, V37, P2046 CAPLUS
- (14) Hartwig, J; J Org Chem 1999, V64, P5575 CAPLUS
- (15) Hartwig, J; J Org Chem 1999, V64, P5575 CAPLUS
- (16) Hayashi, T; Tetrahedron Lett 1988, V29, P99 CAPLUS
- (17) Jegham, S; Tetrahedron Lett 1998, V39, P4453 CAPLUS
- (18) Job, G; Org Lett 2002, V4, P3703 CAPLUS
- (19) Kametani, T; Heterocycles 1980, V14, P277 CAPLUS
- (20) Kawatsura, M; J Am Chem Soc 1999, V121, P1473 CAPLUS
- (21) Keane, P; J Pharm Pharmacol 1979, V31, P752 CAPLUS
- (22) Klapars, A; J Am Chem Soc 2001, V123, P7727 CAPLUS
- (23) Kranenburg, M; Organometallics 1995, V14, P3081 CAPLUS
- (24) Larksarp, C; J Am Chem Soc 1997, V119, P3709 CAPLUS
- (25) Lindley, J; Tetrahedron 1984, V40, P1435
- (26) Madar, D; Tetrahedron Lett 2001, V42, P3681 CAPLUS
- (27) Mai, A; J Med Chem 2002, V45, P1180 CAPLUS
- (28) Moreno-Manas, M; Eur J Org Chem 1999, P181 CAPLUS
- (29) Moureau, F; Eur J Med Chem 1992, V27, P939 CAPLUS
- (30) Moureau, F; Eur J Med Chem 1994, V29, P269 CAPLUS
- (31) Nicolaou, K; Angew Chem, Int Ed 2000, V39, P625 CAPLUS
- (32) Schaus, S; Tetrahedron Lett 1996, V37, P7937 CAPLUS
- (33) Shakespeare, W; Tetrahedron Lett 1999, V40, P2035 CAPLUS
- (34) Trost, B; J Am Chem Soc 1988, V110, P7933 CAPLUS
- (35) Tucker, J; J Med Chem 1998, V41, P3727 CAPLUS
- (36) Wagaw, S; J Am Chem Soc 1999, V121, P10251 CAPLUS
- (37) Wang, Z; Tetrahedron Lett 1999, V40, P3543 CAPLUS
- (38) Wolfe, J; Acc Chem Res 1998, V31, P805 CAPLUS
- (39) Wolfe, J; J Org Chem 2000, V65, P1144 CAPLUS
- (40) Wolfe, J; J Org Chem 2000, V65, P1158 CAPLUS
- (41) Wolfe, J; Tetrahedron 1996, V21, P7525
- (42) Wolfe, J; Tetrahedron 1996, V52, P7525 CAPLUS
- (43) Yang, B; J Organomet Chem 1999, V576, P125 CAPLUS
- (44) Yang, B; Org Lett 1999, V1, P35 CAPLUS
- (45) Yin, J; J Am Chem Soc 2002, V124, P6043 CAPLUS
- (46) Yin, J; Org Lett 2000, V2, P1101 CAPLUS

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FILE LAST UPDATED: 20 Jan 2005 (20050120/ED)

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L4 3 L3

=> d L4 ibib abs hitstr 1-3

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:390234 CAPLUS

DOCUMENT NUMBER: 140:406800

TITLE: Methods for preparing N-aryl oxazolidinones via a copper catalyzed cross coupling reaction

INVENTOR(S): Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

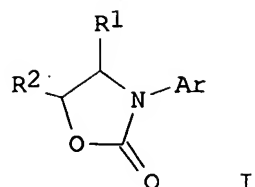
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039788	A1	20040513	WO 2003-IB4708	20031022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004122226	A1	20040624	US 2003-645779	20030821
PRIORITY APPLN. INFO.:			US 2002-423328P	P 20021101
			US 2003-645779	A 20030821
OTHER SOURCE(S):		MARPAT 140:406800		
GI				

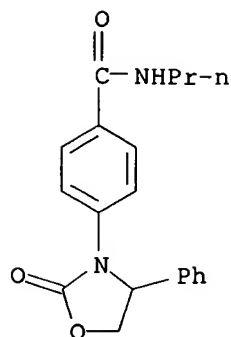


AB Methods for the preparation of N-aryl oxazolidinones (shown as I; variables defined below; e.g. (R)-4-ethyl-3-(4-trifluoromethylphenyl)oxazolidin-2-one (II)) via a Cu catalyzed cross coupling reaction are disclosed. These compds. are intermediates useful in the preparation of cholesteryl ester transfer protein inhibitors. Preferred catalyst ligands are MeNHCH<sub>2</sub>CH<sub>2</sub>NHMe and 1,2-diaminocyclohexane. For example, II was prepared by charging K<sub>2</sub>CO<sub>3</sub> (87 mmol) and CuI (4.4 mmol) to a flask under N<sub>2</sub> and adding (R)-4-ethyloxazolidin-2-one (43.5 mmol) and 1-bromo-4-trifluoromethylbenzene (42.8 mmol) each diluted in 20 mL dioxane to the flask followed by 1,2-diaminocyclohexane (4.4 mmol); the bright blue mixture was heated to 110° and held for 22 h; workup gave 86 % product. Further examples describe the conversion of II to (R)-2-(4-trifluoromethylphenylamino)butan-1-ol (97 %), (R)-4-ethyl-3-(4-trifluoromethylphenyl)-[1,2,3]oxathiazolidine 2-oxide (81 %) and finally (R)-3-(4-trifluoromethylphenylamino)pentanenitrile (81 %). Six addnl. examples of preparation of I are included. For I: R<sub>1</sub> is a partially saturated, fully saturated or fully unsatd. (C1-C4) straight or branched C chain wherein the carbons, other than the connecting C, may optionally be replaced with one heteroatom = O, S and N wherein said C atoms are optionally mono, di- or trisubstituted independently with halo, said C is optionally monosubstituted with oxo or hydroxy, said S is optionally mono- or disubstituted with oxo, said N is optionally mono- or disubstituted with oxo; or said R<sub>1</sub> is a partially saturated, fully saturated or fully unsatd. 3-5-membered ring optionally having one heteroatom = O, S and N; wherein said R<sub>1</sub> ring is optionally mono, di- or trisubstituted independently with halo, (C1-C6)alkoxy, nitro, (C1-C4)alkyloxycarbonyl. R<sub>2</sub> is H, C1-C4 alkyl, C3-C6 cycloalkyl, C2-C6 alkenyl, C2-C6 alkynyl, C1-C4 alkoxy, C1-C4 alkoxy-C1-C4 alkyl; Ph (un)substituted with C1-C6 alkoxy or OY wherein Y is a hydroxy protecting group, halogen, C1-C4 alkyl, C2-C6 alkenyl, C2-C6 alkynyl, C1-C4 alkoxy, C1-C4 alkoxy-C1-C4 alkyl, trifluoromethyl, nitro, carbo-C1-C4 alkoxy, C1-C4 alkoxy carbonyl, carbonyl, or cyano; or benzyl with the Ph moiety of the benzyl (un)substituted with C1-C6 alkoxy or OY wherein Y is a hydroxy protecting group, halogen, C1-C4 alkyl, C2-C6 alkenyl, C2-C6 alkynyl, C1-C4 alkoxy-C1-C4 alkyl, trifluoromethyl, amido, nitro, carbo-C1-C4 alkoxy, C1-C4 alkoxy carbonyl, carbonyl or cyano; wherein Ar is an aromatic hydrocarbon or heteroarom. moiety Ph, naphthyl, pyridyl, thiophenyl, furanyl, pyrrolyl and pyrimidyl, imidazolyl, oxazolyl, thiazolyl, triazolyl, pyrazolyl, pyrazinyl, pyridazinyl each of which may be (un)substituted by ≥1, preferably 1-2, substituents = halo, hydroxy, C1-C4 alkyl, C2-C6 alkenyl, C2-C6 alkynyl, C1-C4 alkoxy, C1-C4 alkoxy-C1-C4 alkyl, CF<sub>3</sub>, amino, amido, imines, nitro, carbo-C1-C4 alkoxy, C1-C4 alkoxy carbonyl, carbonyls (ketones and aldehydes), cyano.

IT **686347-72-8P**, 3-[4-[(Propylamino)carbonyl]phenyl]-4-phenyloxazolidin-2-one  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (methods for preparing N-aryl oxazolidinones via copper catalyzed cross coupling reaction)

RN 686347-72-8 CAPLUS

CN Benzamide, 4-(2-oxo-4-phenyl-3-oxazolidinyl)-N-propyl- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:390231 CAPLUS

DOCUMENT NUMBER: 140:391196

TITLE: Process for the preparation of pyrrolidinyl ethylamine compounds via a copper-mediated aryl amination

INVENTOR(S): Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039785	A1	20040513	WO 2003-IB4676	20031022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004152896	A1	20040805	US 2003-699106	20031031
PRIORITY APPLN. INFO.:			US 2002-423328P	P 20021101
OTHER SOURCE(S):			MARPAT 140:391196	
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention provides a new process for the preparation of the well-known kappa agonists I via a copper salt-catalyzed amination of an oxazolidinone II with an aryl halide III in the presence of an amino ligand and a base [wherein A = H, OH and derivs., fluoro/alkyl, etc.; Ar1 = (un)substituted phenyl; Ar2 = (un)substituted Ph, naphthyl, pyridinyl, thiophenyl, furyl, pyrrolyl, pyrimidinyl; R1 = alkyl, benzyl, with its Ph part optionally substituted; R2, R3 = independently H, (un)substituted alkyl, or R2R3N = (un)substituted pyrrolidine, piperidine, morpholine; X = Cl, Br, I]. The advantages of the aryl amination include high yields, mild, efficient, cost-effective and robust process. For example, aryl amination of S-(+)-4-phenyloxazolidin-2-one with 4-bromo-N-propylbenzamide in the

presence of CuI/K<sub>2</sub>CO<sub>3</sub> gave the intermediate IV, used in the synthesis of pyrrolidinyl ethylamine V.

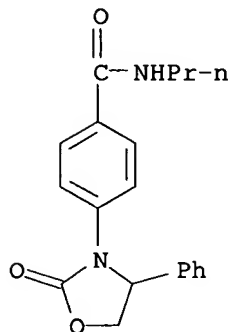
IT 686347-72-8P, 4-(2-Oxo-4-phenyloxazolidin-3-yl)-N-propylbenzamide  
686347-74-0P, 4-(2-Oxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide 686347-75-1P, 4-(2,2-Dioxo-4-phenyl-[1,2,3]oxathiazolidin-3-yl)-N-propylbenzamide

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

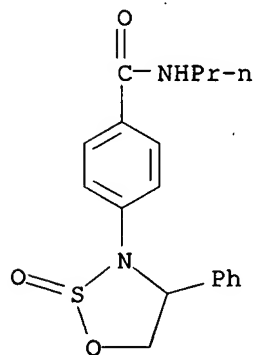
RN 686347-72-8 CAPLUS

CN Benzamide, 4-(2-oxo-4-phenyl-3-oxazolidinyl)-N-propyl- (9CI) (CA INDEX NAME)



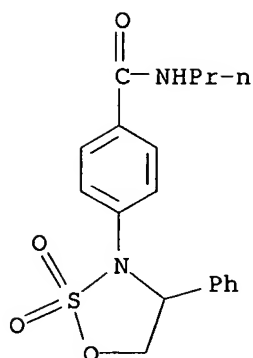
RN 686347-74-0 CAPLUS

CN Benzamide, 4-(2-oxido-4-phenyl-1,2,3-oxathiazolidin-3-yl)-N-propyl- (9CI) (CA INDEX NAME)



RN 686347-75-1 CAPLUS

CN Benzamide, 4-(2,2-dioxido-4-phenyl-1,2,3-oxathiazolidin-3-yl)-N-propyl- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:397213 CAPLUS

DOCUMENT NUMBER: 139:149559

TITLE: Palladium-Catalyzed Synthesis of N-Aryloxazolidinones from Aryl Chlorides

AUTHOR(S): Ghosh, Arun; Sieser, Janice E.; Riou, Maxime; Cai, Weiling; Rivera-Ruiz, Luis

CORPORATE SOURCE: Process Research and Development, Pfizer Global Research and Development, Groton, CT, 06340-8013, USA

SOURCE: Organic Letters (2003), 5(13), 2207-2210

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:149559

AB An efficient method for intermol. N-arylation of oxazolidinones using Pd2dba3 and various phosphine ligands in the presence of a weak base is reported. The conditions allow the use of cheaper aryl chlorides containing functionalities such as enolizable ketones, amides, etc., which would be incompatible with other coupling methods. The coupling reaction can be used to prepare enantiopure N-aryl  $\beta$ -amino alcs. Depending on the stereoelectronic nature of the aryl chloride, careful choice of ligand was necessary for the success of these reactions.

IT **572923-17-2P**

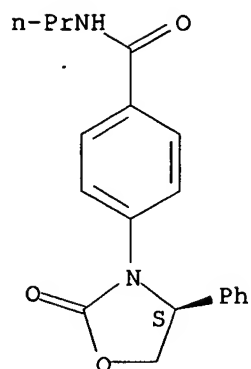
RL: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)

RN 572923-17-2 CAPLUS

CN Benzamide, 4-[(4S)-2-oxo-4-phenyl-3-oxazolidinyl]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

*have this*



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
15.27	202.92

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-2.19	-4.91

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Jan 14, 2005 (20050114/UP).

=> fil beilstein

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.06	202.98

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-4.91

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FILE RELOADED ON OCTOBER 20, 2002  
FILE LAST UPDATED ON NOVEMBER 3, 2004

FILE COVERS 1771 TO 2004.  
\*\*\* FILE CONTAINS 9,073,068 SUBSTANCES \*\*\*

>>>PLEASE NOTE: Reaction Data and substance data are stored in  
separate documents and can not be searched together in one query.  
Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes 'PRE (preparations) and REA  
(reactions). A substance answer set retrieved after the search  
for a chemical name, a compounds with available reaction  
information by combining with PRE/FA, REA/FA or more generally

with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

**NEW**

\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=> s L4  
L5 0 L3

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.14	203.12
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.91

FILE 'CAOLD' ENTERED AT 19:21:15 ON 21 JAN 2005  
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FILE COVERS 1907-1966  
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s L4  
L6 0 L3

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.43	203.55
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.91

FILE 'CASREACT' ENTERED AT 19:21:49 ON 21 JAN 2005  
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FILE CONTENT:1840 - 16 Jan 2005 VOL 141 ISS 20

```
*****
*
*      CASREACT now has more than  8 million reactions      *
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s L4
L7          1 L3
```

```
=> d L7 ibib abs hitstr
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'
```

The following are valid formats:

```
ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE, Single-step Reactions
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
DALL ----- ALL, delimited (end of each field identified)
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IND ----- Indexing data
IPC ----- International Patent Classifications
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

MAX ----- Same as ALL
PATS ----- PI, SO
SCAN ----- TI and FCRD (random display, no answer number.  SCAN
                  must be entered on the same line as DISPLAY, e.g.,
                  D SCAN.)
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for
                  all single-step reactions)
STD ----- BIB, IPC, and NCL

CRD ----- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
```



FHIT ----- Reaction Map, Diagram, and Summary for first  
 hit reaction  
 FHITCBIB --- FHIT, AN plus CBIB  
 FCRD ----- First hit in Compact Reaction Display (CRD) format  
 FCRDREF ---- First hit in Compact Reaction Display (CRD) format with  
 CA reference information (SO, PY). (Default)  
 FPATH ----- PATH, plus Reaction Summary for the "long path"  
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
 HIT ----- Reaction Map, Reaction Diagram, and Reaction  
 Summary for all hit reactions and fields containing  
 hit terms  
 OCC ----- All hit fields and the number of occurrences of the  
 hit terms in each field. Includes total number of  
 HIT, PATH, SPATH reactions. Labels reactions that have  
 incomplete verifications.  
 PATH ----- Reaction Map and Reaction Diagram for the "long  
 path". Displays all hit reactions, except those  
 whose steps are totally included within another hit  
 reaction which is displayed  
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
 RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
 SPATH ----- Reaction Map and Reaction Diagram for the "short  
 path". Displays all single step reactions which  
 contain a hit substance. Also displays those  
 multistep reactions that have a hit substance in both  
 the first and last steps of the reaction, except for  
 those hit reactions whose steps are totally included  
 within another hit reaction which is displayed

To display a particular field or fields, enter the display field  
 codes. For a list of the display field codes, enter HELP DFIELDS  
 at an arrow prompt (=>). Examples of combinations include: D TI;  
 D BIB RX; D TI, AU, FCRD. The information is displayed in the same order  
 as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,  
 FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may  
 be used with the DISPLAY command to display the record for a specified  
 Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):ibib

L7 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 139:149559 CASREACT  
 TITLE: Palladium-Catalyzed Synthesis of N-Aryloxazolidinones  
 from Aryl Chlorides  
 AUTHOR(S): Ghosh, Arun; Sieser, Janice E.; Riou, Maxime; Cai,  
 Weiling; Rivera-Ruiz, Luis  
 CORPORATE SOURCE: Process Research and Development, Pfizer Global  
 Research and Development, Groton, CT, 06340-8013, USA  
 SOURCE: Organic Letters (2003), 5(13), 2207-2210  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y  
 COST IN U.S. DOLLARS

SINCE FILE TOTAL  
 ENTRY SESSION

FULL ESTIMATED COST

29.16

232.71

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-4.91

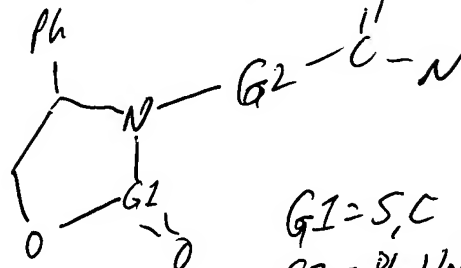
STN INTERNATIONAL LOGOFF AT 19:22:45 ON 21 JAN 2005

Connecting via Winsock to STN

106991069

1/21/05

Structure search



Welcome to STN International! Enter x:x

LOGINID:SSSPTAAJP1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\*\*\*\*\* Welcome to STN International \*\*\*\*\*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 SEP 01 New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!  
NEWS 4 OCT 28 KOREAPAT now available on STN  
NEWS 5 NOV 30 PHAR reloaded with additional data  
NEWS 6 DEC 01 LISA now available on STN  
NEWS 7 DEC 09 12 databases to be removed from STN on December 31, 2004  
NEWS 8 DEC 15 MEDLINE update schedule for December 2004  
NEWS 9 DEC 17 ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 10 DEC 17 COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 11 DEC 17 SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 12 DEC 17 CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected  
NEWS 13 DEC 17 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB  
NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN  
NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED  
NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and February 2005  
NEWS 17 JAN 11 CA/CAPLUS - Expanded patent coverage to include Russia (Federal Institute of Industrial Property)  
  
NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

0 hits  
CAW  
CAPLUS  
Cmpl (VI)

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FILE 'HOME' ENTERED AT 19:09:19 ON 21 JAN 2005

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 19:09:28 ON 21 JAN 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

DICTIONARY FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

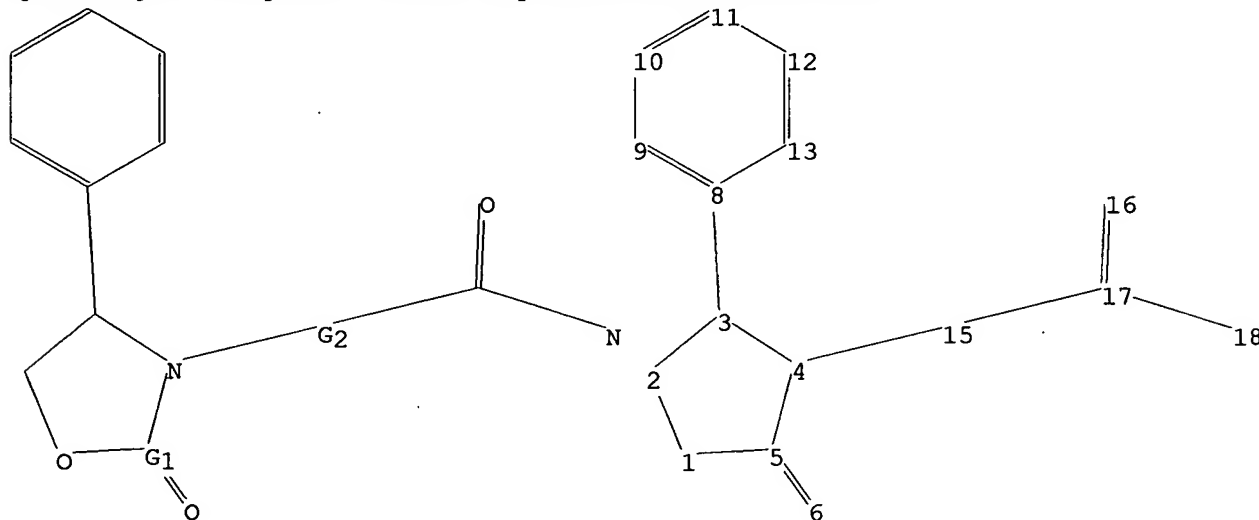
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10699106c.str



chain nodes :

6 15 16 17 18

ring nodes :

1 2 3 4 5 8 9 10 11 12 13

chain bonds :

3-8 4-15 5-6 15-17 16-17 17-18

ring bonds :

1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13

exact/norm bonds :

1-2 1-5 2-3 3-4 3-8 4-5 4-15 5-6 15-17 16-17 17-18

normalized bonds :

8-9 8-13 9-10 10-11 11-12 12-13

G1:C,S

G2:Ph,Hy

Match level :

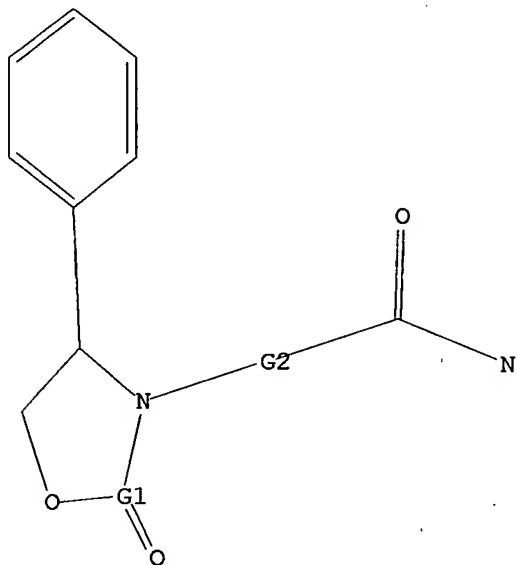
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 C,S

G2 Ph,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s L1

SAMPLE SEARCH INITIATED 19:10:02 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 299 TO ITERATE

100.0% PROCESSED 299 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 4943 TO 7017

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 19:10:07 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5770 TO ITERATE

100.0% PROCESSED 5770 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L3 0 SEA SSS FUL L1

=> fil casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

162.19

162.40

FILE 'CASREACT' ENTERED AT 19:11:12 ON 21 JAN 2005  
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FILE CONTENT:1840 - 16 Jan 2005 VOL 141 ISS 20

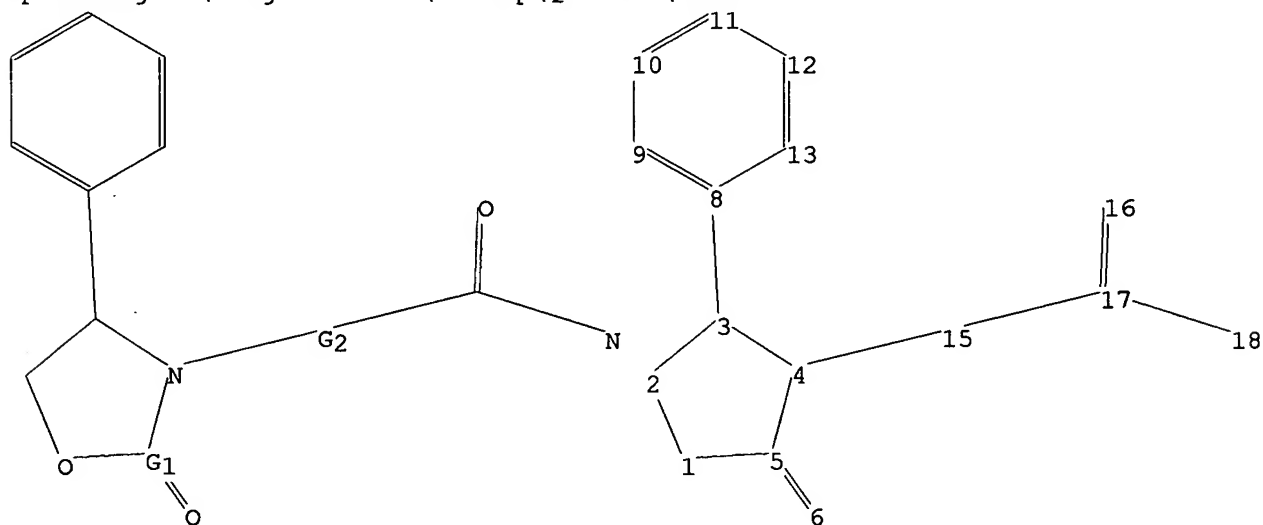
\*\*\*\*\*  
\*  
\* CASREACT now has more than 8 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10699106c.str



chain nodes :

6 15 16 17 18

ring nodes :

1 2 3 4 5 8 9 10 11 12 13

chain bonds :

3-8 4-15 5-6 15-17 16-17 17-18  
 ring bonds :  
 1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13  
 exact/norm bonds :  
 1-2 1-5 2-3 3-4 3-8 4-5 4-15 5-6 15-17 16-17 17-18  
 normalized bonds :  
 8-9 8-13 9-10 10-11 11-12 12-13

G1:C,S

G2:Ph,Hy

Match level :

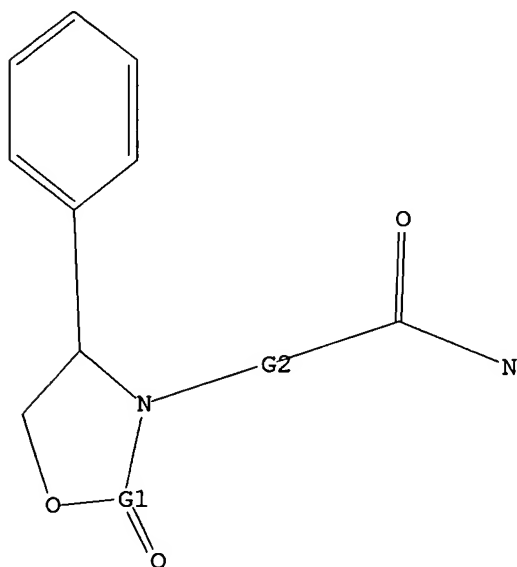
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



G1 C,S

G2 Ph,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s L4

SAMPLE SEARCH INITIATED 19:11:37 FILE 'CASREACT'

SCREENING COMPLETE - 440 REACTIONS TO VERIFY FROM 26 DOCUMENTS

100.0% DONE 440 VERIFIED 0 HIT RXNS

0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 7543 TO 10057  
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4 ( 0 REACTIONS)

=> s L4 full

FULL SEARCH INITIATED 19:11:45 FILE 'CASREACT'

SCREENING COMPLETE - 10457 REACTIONS TO VERIFY FROM 585 DOCUMENTS

100.0% DONE 10457 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4 ( 0 REACTIONS)

=> index structure

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
106.53	268.93

FULL ESTIMATED COST

INDEX 'BEILSTEIN, CASREACT, CHEMINFORMRX, DJSMONLINE, DRUGU, GMELIN, MARPAT,  
MARPATPREV, PS, REGISTRY' ENTERED AT 19:11:57 ON 21 JAN 2005

10 FILES IN THE FILE LIST IN STNINDEX

Enter SET DETAIL ON to see search term postings or to view  
search error messages that display as 0\* with SET DETAIL OFF.

=> s L4

SUBSTANCE SEARCHES NOT VALID IN INDEX

Substance searches are not available in index.

=> fil gmelin

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.59	269.52

FULL ESTIMATED COST

FILE 'GMELIN' ENTERED AT 19:12:14 ON 21 JAN 2005

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FILE LAST UPDATED: 03 MAY 97 - 21 MAY 97 <970503/UP -970521/UP>

>>> CAS REGISTRY NUMBERS FOR 171,499 SUBSTANCES AVAILABLE <<<

>>> FILE CONTAINS 1,070,350 SUBSTANCES <<<

>>> PLEASE NOTE THAT AFTER A SEARCH IN SSTA FIELDS DIS QRD OR  
DIS HIT CAN BE VERY LENGTHY. <<<

\*\*\*\*\*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR PREDEFINED \*  
\* FORMATS ARE BASED ON THE SUM OF ALL FIELDS POSSIBLE. THEREFORE; \*  
\* THESE ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST. \*  
\*\*\*\*\*

=> s L4

SAMPLE SEARCH INITIATED 19:12:18 FILE 'GMELIN'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*



BATCH      \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:      0 TO      0  
PROJECTED ANSWERS:      0 TO      0

L7              0 SEA SSS SAM L4

=> s L4 full

FULL SEARCH INITIATED 19:12:30 FILE 'GMELIN'

FULL SCREEN SEARCH COMPLETED -      11 TO ITERATE

100.0% PROCESSED      11 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.03

L8              0 SEA SSS FUL L4

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

15.02

284.54

STN INTERNATIONAL LOGOFF AT 19:13:09 ON 21 JAN 2005

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1/21/05  
106991066.

Welcome to STN International! Enter x:x

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2



\* \* \* \* \* Welcome to STN International \* \* \* \* \*

7 of 7

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	JAN 11	CA/CAPLUS - Expanded patent coverage to include Russia (Federal Institute of Industrial Property)
NEWS EXPRESS			JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 18:15:09 ON 21 JAN 2005

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 18:15:29 ON 21 JAN 2005

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STRUCTURE FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

DICTIONARY FILE UPDATES: 19 JAN 2005 HIGHEST RN 817158-90-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

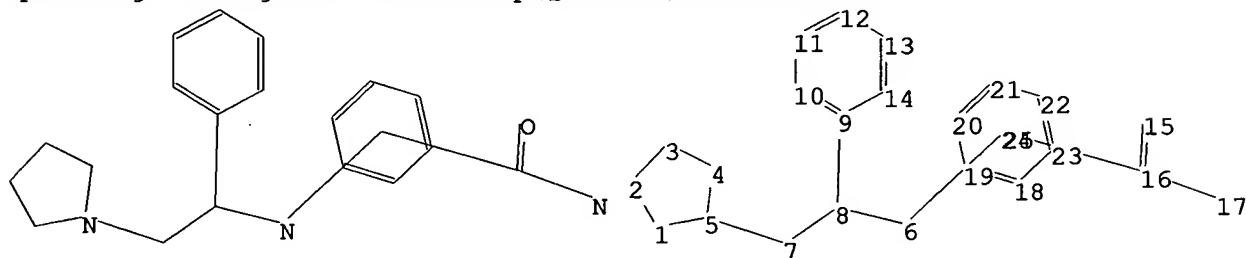
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10699106a.str



chain nodes :

6 7 8 15 16 17

ring nodes :

1 2 3 4 5 9 10 11 12 13 14 18 19 20 21 22 23

chain bonds :

5-7 6-8 7-8 8-9 15-16 16-17

ring bonds :

1-2 1-5 2-3 3-4 4-5 9-10 9-14 10-11 11-12 12-13 13-14 18-19 18-23  
19-20 20-21 21-22 22-23

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 5-7 6-8 15-16 16-17

exact bonds :

7-8 8-9

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14 18-19 18-23 19-20 20-21 21-22 22-23

Match level :

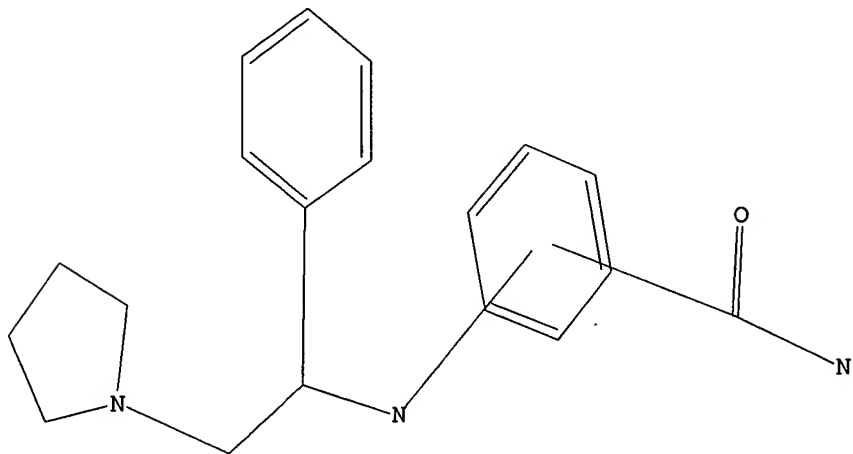
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom  
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L1

SAMPLE SEARCH INITIATED 18:15:53 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1356 TO ITERATE

73.7% PROCESSED 1000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

7 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 24911 TO 29329  
PROJECTED ANSWERS: 7 TO 373

L2 7 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 18:16:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 26680 TO ITERATE

100.0% PROCESSED 26680 ITERATIONS  
SEARCH TIME: 00.00.01

147 ANSWERS

L3 147 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY      SESSION  
161.33      161.54

FILE 'CAPLUS' ENTERED AT 18:16:08 ON 21 JAN 2005  
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FILE COVERS 1907 - 21 Jan 2005 VOL 142 ISS 5  
FILE LAST UPDATED: 20 Jan 2005 (20050120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3

L4                      7 L3

=> d L4 ibib abs hitstr 1-7

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:      2004:390231 CAPLUS

DOCUMENT NUMBER:      140:391196

TITLE:                      Process for the preparation of pyrrolidinyl ethylamine compounds via a copper-mediated aryl amination

INVENTOR(S):              Caron, Stephane; Ghosh, Arun; Sieser, Janice Ethel

PATENT ASSIGNEE(S):      Pfizer Products Inc., USA

SOURCE:                      PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE:              Patent

LANGUAGE:                      English

FAMILY ACC. NUM. COUNT:    2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039785	A1	20040513	WO 2003-IB4676	20031022
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2004152896	A1	20040805	US 2003-699106	20031031
PRIORITY APPLN. INFO.:			US 2002-423328P	P 20021101
OTHER SOURCE(S):	MARPAT	140:391196		
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

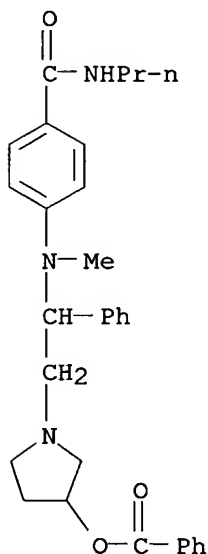
AB The invention provides a new process for the preparation of the well-known kappa agonists I via a copper salt-catalyzed amination of an oxazolidinone II with an aryl halide III in the presence of an amino ligand and a base [wherein A = H, OH and derivs., fluoro/alkyl, etc.; Ar1 = (un)substituted phenyl; Ar2 = (un)substituted Ph, naphthyl, pyridinyl, thiophenyl, furyl, pyrrolyl, pyrimidinyl; R1 = alkyl, benzyl, with its Ph part optionally substituted; R2, R3 = independently H, (un)substituted alkyl, or R2R3N = (un)substituted pyrrolidine, piperidine, morpholine; X = Cl, Br, I]. The advantages of the aryl amination include high yields, mild, efficient, cost-effective and robust process. For example, aryl amination of S-(+)-4-phenyloxazolidin-2-one with 4-bromo-N-propylbenzamide in the presence of CuI/K2CO3 gave the intermediate IV, used in the synthesis of pyrrolidinyl ethylamine V.

IT **686347-77-3P**, Benzoic acid 1-[2-[methyl[4-(propylcarbamoyl)phenyl]amino]-2-phenylethyl]pyrrolidin-3-yl ester  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(amine product; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

RN 686347-77-3 CAPLUS

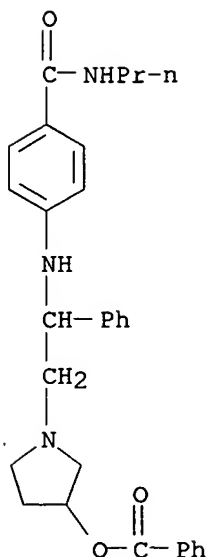
CN Benzamide, 4-[[2-[3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)



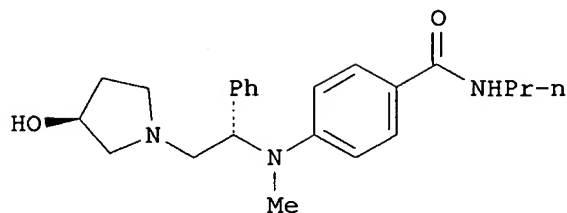
IT **686347-76-2P**, Benzoic acid 1-[2-phenyl-2-[[4-(propylcarbamoyl)phenyl]amino]ethyl]pyrrolidin-3-yl ester  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; process for preparation of pyrrolidinyl ethylamines via a copper-mediated aryl amination)

RN 686347-76-2 CAPLUS

CN Benzamide, 4-[[2-[3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:877272 CAPLUS  
 DOCUMENT NUMBER: 140:111217  
 TITLE: Efficient synthesis of the  $\kappa$ -opioid receptor agonist CJ-15,161: four stereospecific inversions at a single aziridinium stereogenic center  
 AUTHOR(S): Couturier, Michel; Tucker, John L.; Andresen, Brian M.; DeVries, Keith M.; Vanderplas, Brian C.; Ito, Fumitaka  
 CORPORATE SOURCE: Chemical Research & Development, Pfizer Inc., Groton, CT, 06340, USA  
 SOURCE: Tetrahedron: Asymmetry (2003), 14(22), 3517-3523  
 CODEN: TASYE3; ISSN: 0957-4166  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 140:111217  
 GI



I

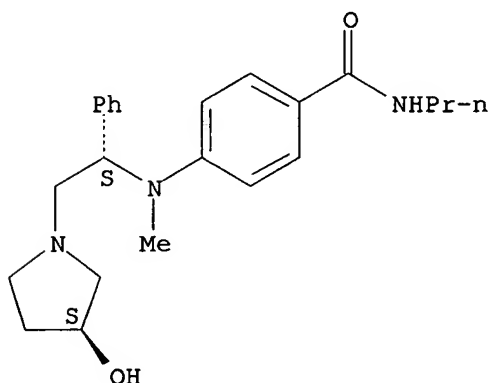
AB An efficient four-step sequence has been developed for the synthesis of the  $\kappa$ -opioid receptor agonist I (CJ-15,161). The process features four consecutive regioselective and stereospecific inversions at a single aziridinium stereogenic center, which leads to overall retention of stereochem., in a single operation. The chemical is straightforward, practical and amenable to large-scale synthesis. Crystal structure of suitable for formulation polymorph benzoate salt form of I is also reported.

IT **646041-98-7**  
 RL: PRP (Properties)  
 (crystal structure; large-scale synthesis of  $\kappa$ -opioid receptor  
 agonist, (arylamino)(phenyl)ethyl pyrrolidinol)  
 RN 646041-98-7 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-  
 phenylethyl]methylamino]-N-propyl-, monobenzoate (salt), monohydrate (9CI)  
 (CA INDEX NAME)

CM 1

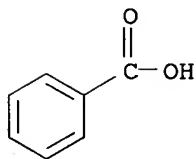
CRN 204970-97-8  
 CMF C23 H31 N3 O2

Absolute stereochemistry. Rotation (+).



CM 2

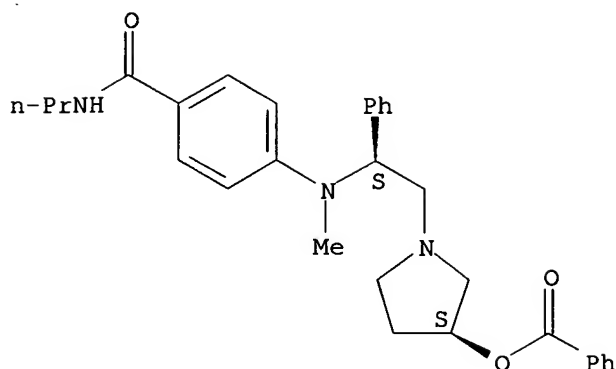
CRN 65-85-0  
 CMF C7 H6 O2



IT **473916-34-6P**  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic  
 preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (large-scale synthesis of  $\kappa$ -opioid receptor agonist,  
 (arylamino)(phenyl)ethyl pyrrolidinol)  
 RN 473916-34-6 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(benzoyloxy)-1-pyrrolidinyl]-1-  
 phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).





IT 204970-97-8P

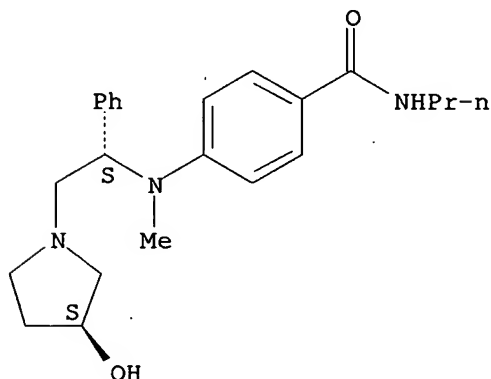
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(large-scale synthesis of  $\kappa$ -opioid receptor agonist, (arylamino)(phenyl)ethyl pyrrolidinol)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:696867 CAPLUS

DOCUMENT NUMBER: 139:230618

TITLE: Preparation of crystalline anhydrous and monohydrate benzoate salts of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine as  $\kappa$ -opioid receptor agonists

INVENTOR(S): Quallich, George Joseph; Castaldi, Michael James

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

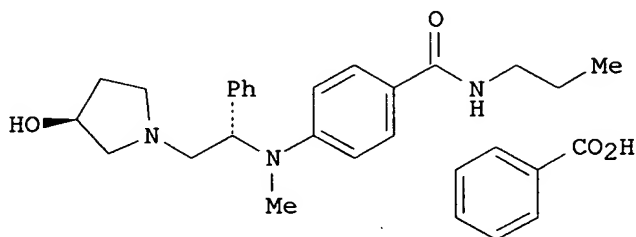
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

possible  
prev. ODP

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072544	A1	20030904	WO 2003-IB560	20030217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1478622	A1	20041124	EP 2003-742880	20030217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004235936	A1	20041125	US 2003-421209	20030423
PRIORITY APPLN. INFO.:			US 2002-360250P	P 20020228
			WO 2003-IB560	W 20030217

GI



I

AB A process for preparing an anhydrous crystalline benzoate salt of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine (I) and the corresponding I crystalline benzoate monohydrate is described which comprises: salifying (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine with benzoic acid in the presence of an alkyl alc. (e.g., 2-propanol), and isolating the anhydrous I salt (X-ray diffraction data is presented). The crystalline monohydrate benzoate salt of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine is prepared by: treating anhydrous I with an aqueous alkanol solution; and isolating the crystallization I monohydrate (X-ray diffraction data is presented). These benzoate salts are selective kappa-receptor agonists, and are useful as analgesics, anesthetics, anti-inflammatory or neuroprotective agents, or in the treatment of arthritis, stroke or functional bowel disease (all no data).

IT 591769-11-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of crystalline anhydrous and monohydrate benzoate salts of (2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]amino-2-phenyl]ethylpyrrolidine as  $\kappa$ -opioid receptor agonists)

RN 591769-11-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, compd. with phenol (1:1) (9CI) (CA

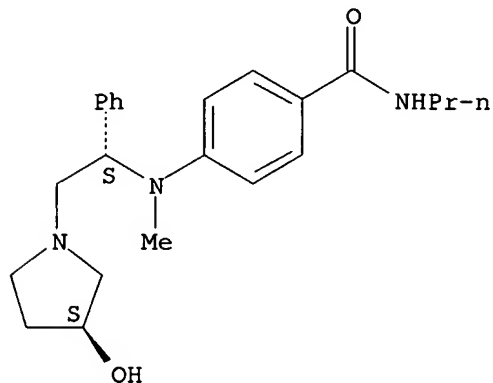
INDEX NAME)

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CRN 204970-97-8

CMF C23 H31 N3 O2

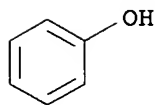
Absolute stereochemistry. Rotation (+).



CM 2

CRN 108-95-2

CMF C6 H6 O



IT 591769-12-9P

RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of crystalline anhydrous and monohydrate benzoate salts of  
(2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]a  
mino-2-phenyl]ethylpyrrolidine as  $\kappa$ -opioid receptor agonists)

RN 591769-12-9 CAPLUS

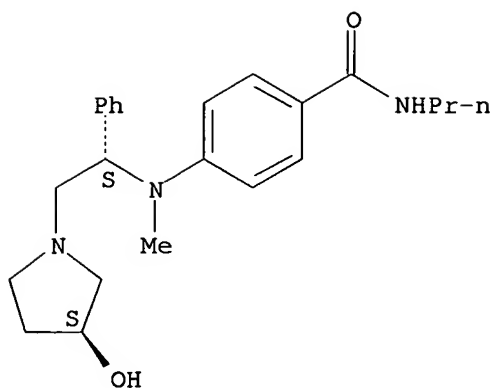
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-  
phenylethyl]methylamino]-N-propyl-, compd. with phenol (1:1), monohydrate  
(9CI) (CA INDEX NAME)

CM 1

CRN 204970-97-8

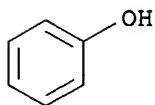
CMF C23 H31 N3 O2

Absolute stereochemistry. Rotation (+).



CM 2

CRN 108-95-2  
CMF C6 H6 O



IT 204970-97-8

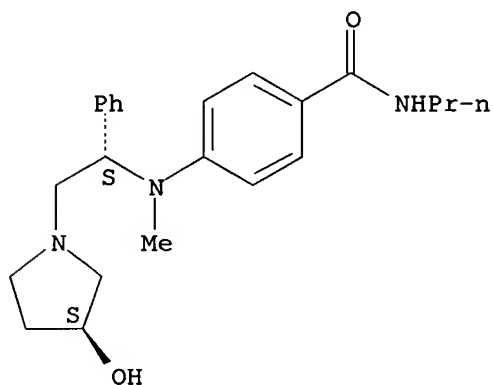
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of crystalline anhydrous and monohydrate benzoate salts of  
(2'S,3S)-3-hydroxy-N-[2-[N-methyl-N-4-[(N-propylamino)carbonyl]phenyl]a  
mino-2-phenyl]ethylpyrrolidine as  $\kappa$ -opioid receptor agonists)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-  
phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:833565 CAPLUS

DOCUMENT NUMBER: 137:337777

TITLE: Preparation of hydroxypyrrolidinyl ethylamine compounds useful as selective  $\kappa$ -opioid receptor agonists

INVENTOR(S): Devries, Keith M.; Couturier, Michel A.; Andresen, Brian M.; Tucker, John L.; Ito, Fumitaka

PATENT ASSIGNEE(S): Pfizer Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 13 pp.  
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002161241	A1	20021031	US 2002-133954	20020426
US 6624313	B2	20030923		
WO 2002088082	A2	20021107	WO 2002-IB924	20020325
WO 2002088082	A3	20040521		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW

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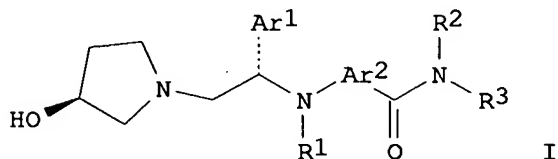
BR 2002009270	A	20040615	BR 2002-9270	20020325
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR

PRIORITY APPLN. INFO.: US 2001-287428P P 20010430  
US 2001-314006P P 20010821  
WO 2002-IB924 W 20020325

OTHER SOURCE(S): CASREACT 137:337777; MARPAT 137:337777

GI

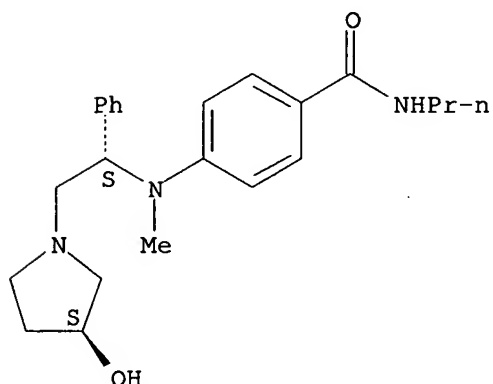


AB Hydroxypyrrolidinyl ethylamine compds. [I; wherein R1 = H, OH, (C1-C4)alkyl, (C1-C4)alkoxy, etc.; R2, R3, independently = H, (C1-C4)alkyl; Ar1, Ar2, independently = aryl, and particularly phenyl] were prepared. For example, (2'S,3S)-3-benzoyloxy-N-{2-[N-methyl-N-4-(N-propylaminocarbonyl)phenyl]amino-2-phenyl}ethylpyrrolidine was prepared by a multistep synthetic procedure. The compds. are useful as selective  $\kappa$ -opioid receptor agonists. In fact, some of the title compds. showed a potent IC50 value against kappa-receptor in the range of 0.01 to 100 nM.

IT **204970-97-8P**  
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of hydroxypyrrolidinyl ethylamine compds. useful as selective

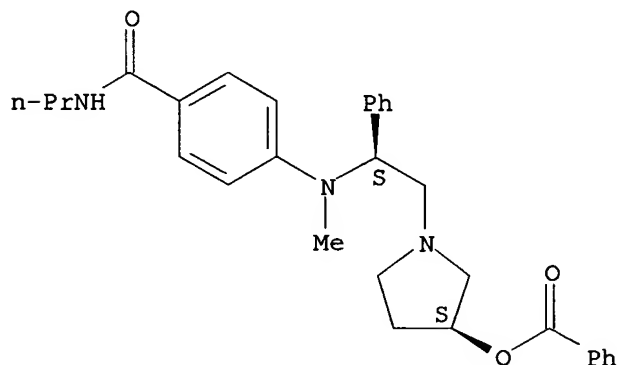
κ-opioid receptor agonists)  
RN 204970-97-8 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 473916-34-6P  
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of hydroxypyrrolidinyl ethylamine compds. useful as selective κ-opioid receptor agonists)  
RN 473916-34-6 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2002:517323 CAPLUS  
DOCUMENT NUMBER: 138:73134  
TITLE: Synthesis of the kappa-agonist CJ-15,161 via a palladium-catalyzed cross-coupling reaction  
AUTHOR(S): Ghosh, Arun; Sieser, Janice E.; Caron, Stephane; Watson, Timothy J. N.  
CORPORATE SOURCE: Chemical Research and Development, Pfizer Global Research and Development, Groton, CT, 06340-8013, USA  
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (15), 1644-1645  
CODEN: CHCOFS; ISSN: 1359-7345  
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 138:73134

AB Syntheses of CJ-15,161 involving intermol. N-arylation of an appropriately functionalized diamine, obtained from the precursor  $\alpha$ -amino acids or, more conveniently, from the corresponding 1,2-amino alcs. via 1,2,3-oxathiazolidine-2,2-dioxide, are reported.

IT **479687-38-2P**

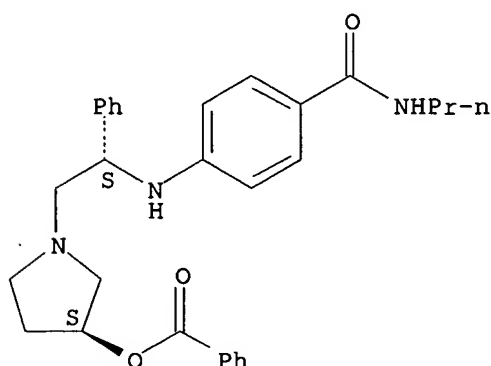
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(formylation of; preparation of kappa-agonist compound via palladium-catalyzed cross-coupling reactions)

RN 479687-38-2 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **473916-34-6P**

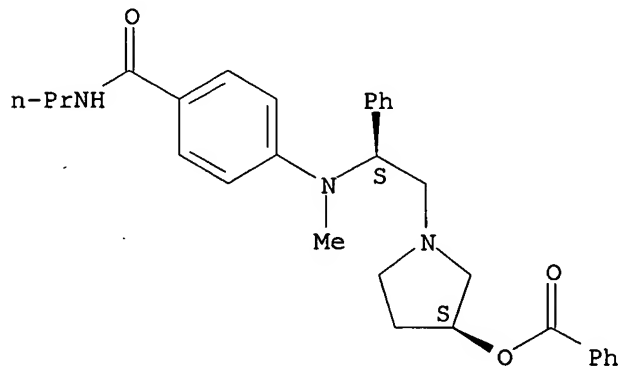
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(hydrolysis of; preparation of kappa-agonist compound via palladium-catalyzed cross-coupling reactions)

RN 473916-34-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(benzoyloxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **204970-97-8P**

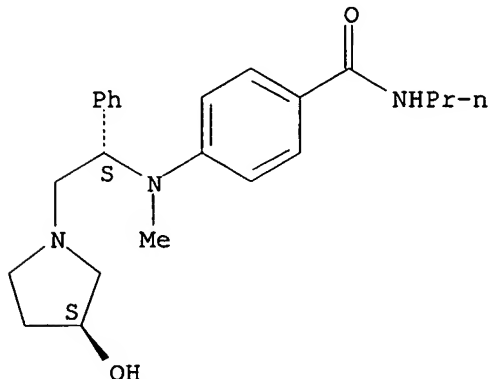
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of kappa-agonist compound via palladium-catalyzed cross-coupling reactions)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:178439 CAPLUS

DOCUMENT NUMBER: 134:222619

TITLE: Preparation of pyrrolidinyl- and pyrrolinylethylarylamines as kappa opioid receptor agonists

INVENTOR(S): Ito, Fumitaka; Kondo, Hiroshi

PATENT ASSIGNEE(S): Pfizer, Inc., USA

SOURCE: U.S., 39 pp., Cont.-in-part of Appl. No. PCT/IB96/00957.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6201007	B1	20010313	US 1999-254805	19990312
WO 9812177	A1	19980326	WO 1997-IB1021	19970821
W: AU, BG, BR, CA, CN, CZ, HU, IL, IS, JP, KR, LK, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
JP 2001316344	A2	20011113	JP 2001-92342	19970821
US 2001008890	A1	20010719	US 2001-770515	20010126
US 6310061	B2	20011030		
US 2001009921	A1	20010726	US 2001-770513	20010126
US 6313302	B2	20011106		
US 2001011091	A1	20010802	US 2001-770514	20010126
US 6294569	B2	20010925		
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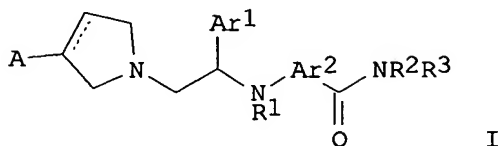


US 6294557  
US 6303602  
PRIORITY APPLN. INFO.:

B2 20010925  
B1 20011016

US 2001-770512 20010126  
WO 1996-IB957 A2 19960918  
WO 1997-IB1021 W 19970821  
JP 1998-514433 A3 19970821  
US 1999-254805 A3 19990312

OTHER SOURCE(S): MARPAT 134:222619  
GI



AB Title compds. [I; A = H, halo, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, O, OY, null; Y = protecting group; broken line = optional double bond; Ar1 = (substituted) Ph; Ar2 = (substituted) Ph, naphththyl, pyridyl, thienyl, furyl, pyrrolyl, pyrimidinyl; R1 = H, OH, alkyl, alkoxy, OY; and R2, R3 = (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, alkoxy, Ph, etc.; R2R3N = (substituted) pyrrolidinyl, piperidinyl, morpholinyl], were prepared as  $\kappa$  agonists (no data). Thus, a mixture of 2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethanol, 2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-2-(R)-phenylethanol (preparation given), and Et3N in CH2Cl2 was treated with MeSO2Cl at 0° followed by 5,5 h stirring at room temperature to give a residue which was refluxed 1.5 h with Me 4-methylaminobenzoate in EtOH to give 62.5% Me 4-[N-[2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethyl]-N-methylamino]benzoate. This was saponified with NaOH in MeOH (quant.) and the acid was stirred with PrNH2 and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride in CH2Cl2 to give 72% Me 4-[N-[2-(3-(S)-methoxymethoxypyrrolidin-1-yl)-1-(S)-phenylethyl]-N-methylamino]-N'-propylbenzamide.

IT 204970-97-8P

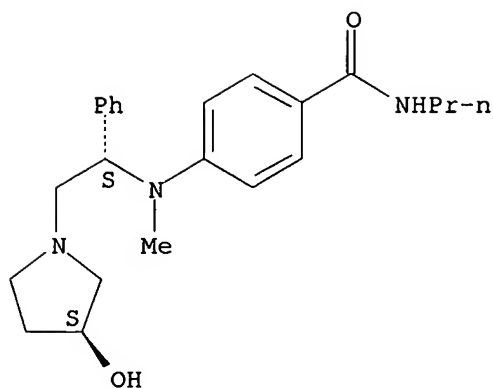
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of pyrrolidinyl- and pyrrolinylethylarylamines as kappa opioid receptor agonists)

RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 204970-95-6P 204970-99-0P 204971-01-7P  
 204971-03-9P 204971-05-1P 204971-07-3P  
 204971-09-5P 204971-11-9P 204971-13-1P  
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 204971-21-1P 204971-23-3P 204971-25-5P  
 204971-27-7P 204971-29-9P 204971-30-2P  
 204971-32-4P 204971-34-6P 204971-36-8P  
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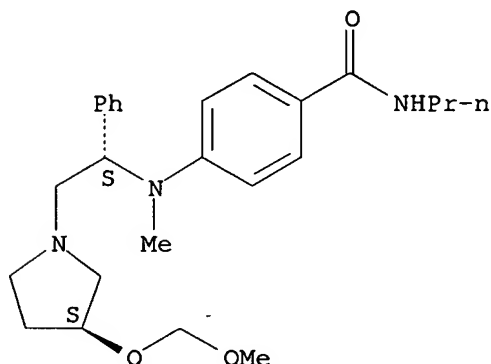
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of pyrrolidinyl- and pyrrolinylethylarylamines as kappa opioid  
receptor agonists)

RN 204970-95-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

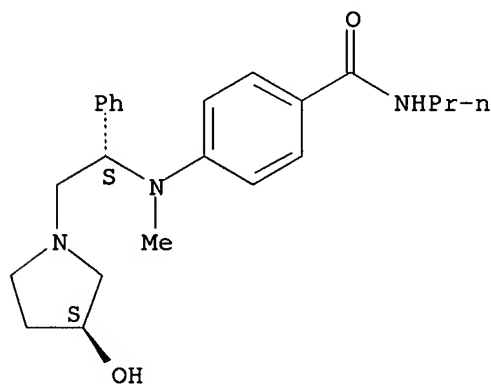
Absolute stereochemistry.



RN 204970-99-0 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

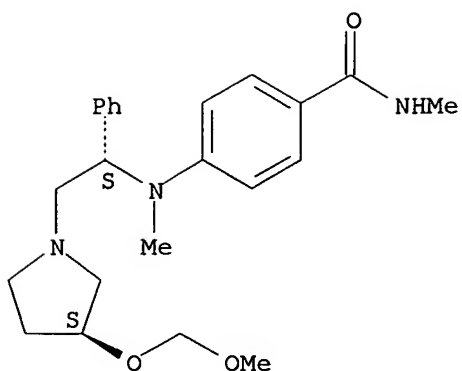


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RN 204971-01-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl- (9CI) (CA INDEX NAME)

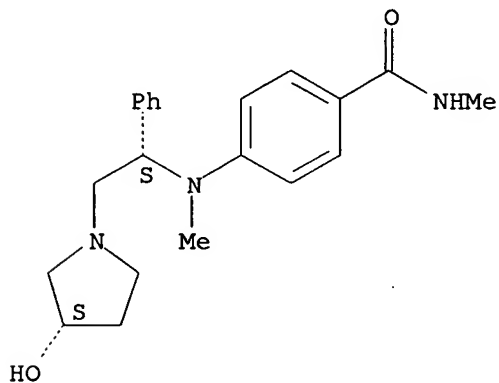
Absolute stereochemistry.



RN 204971-03-9 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl- (9CI) (CA INDEX NAME)

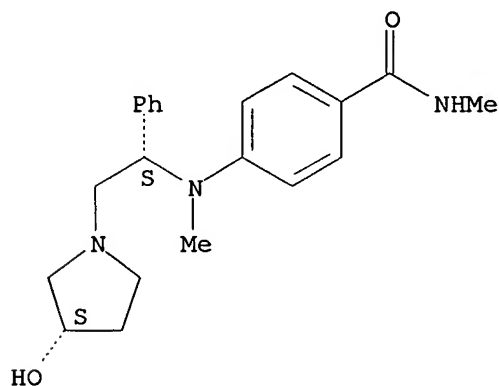
Absolute stereochemistry.



RN 204971-05-1 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

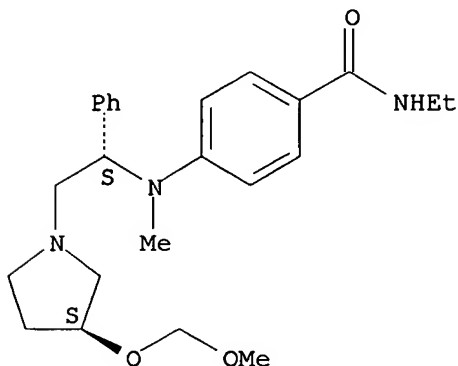


● HCl

RN 204971-07-3 CAPLUS

CN Benzamide, N-ethyl-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

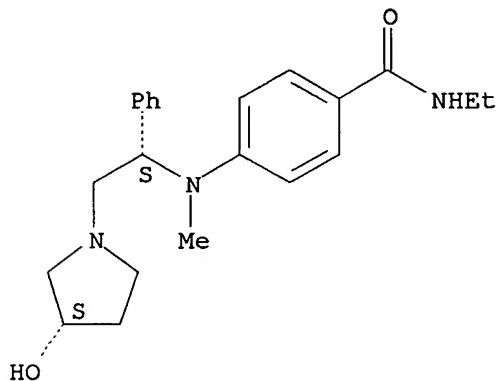
Absolute stereochemistry.



RN 204971-09-5 CAPLUS

CN Benzamide, N-ethyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

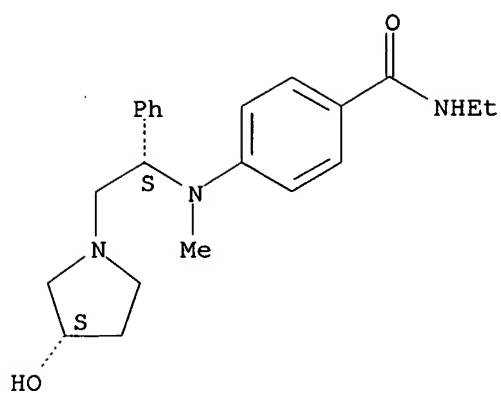
Absolute stereochemistry.



RN 204971-11-9 CAPLUS

CN Benzamide, N-ethyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

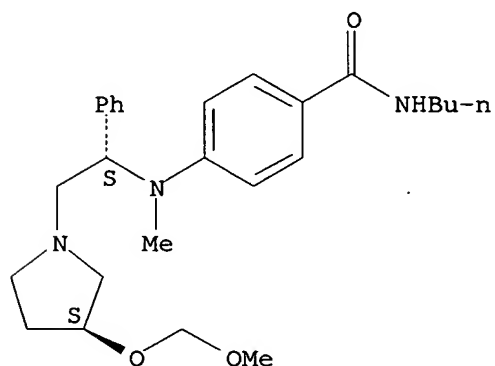


● HCl

RN 204971-13-1 CAPLUS

CN Benzamide, N-butyl-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

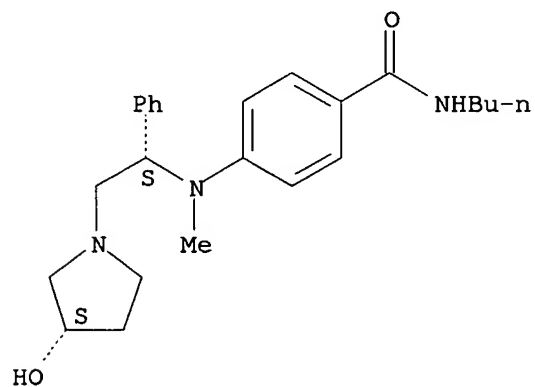
Absolute stereochemistry.



RN 204971-15-3 CAPLUS

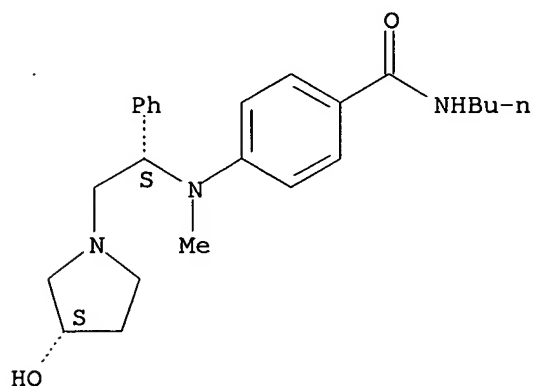
CN Benzamide, N-butyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-17-5 CAPLUS  
CN Benzamide, N-butyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

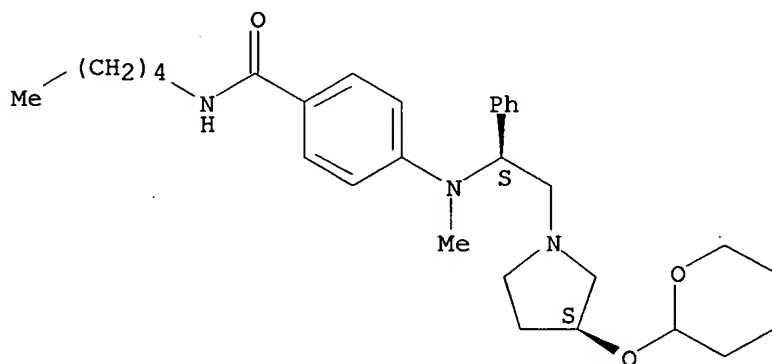
Absolute stereochemistry.



● HCl

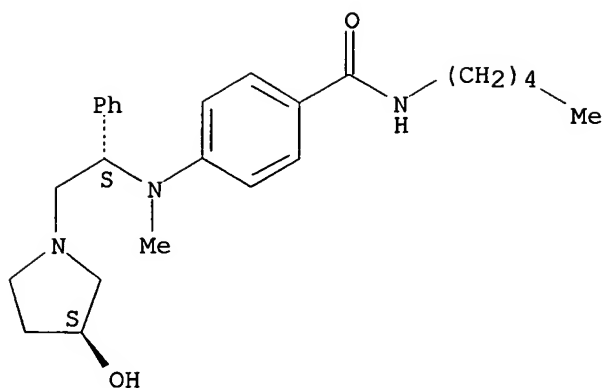
RN 204971-19-7 CAPLUS  
CN Benzamide, 4-[methyl[(1S)-1-phenyl-2-[(3S)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-1-pyrrolidinyl]ethyl]amino]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-21-1 CAPLUS  
CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-pentyl- (9CI) (CA INDEX NAME)

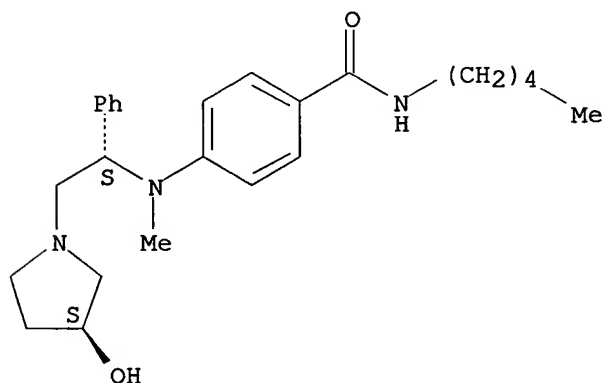
Absolute stereochemistry.



RN 204971-23-3 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-pentyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



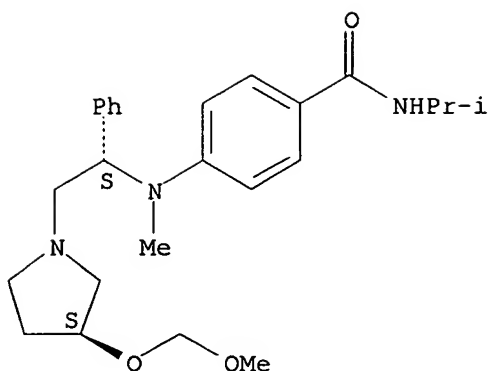
● HCl

RN 204971-25-5 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

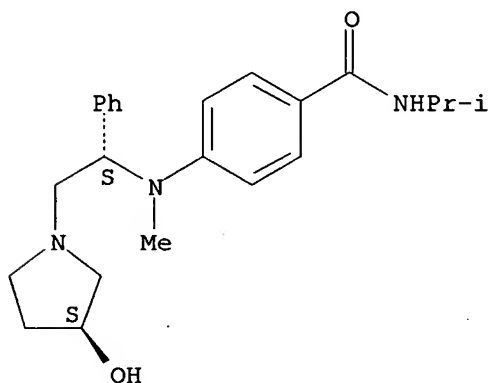




RN 204971-27-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

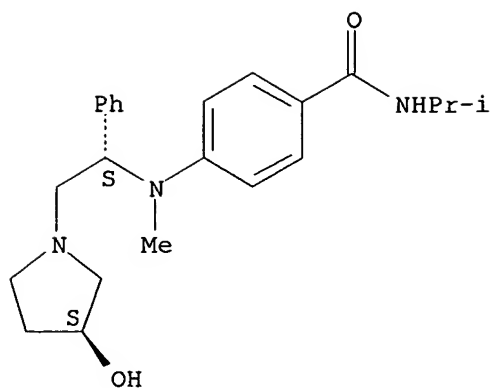
Absolute stereochemistry.



RN 204971-29-9 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(1-methylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

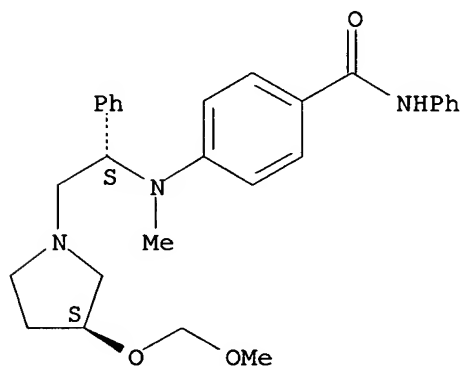


● HCl

RN 204971-30-2 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-phenyl- (9CI) (CA INDEX NAME)

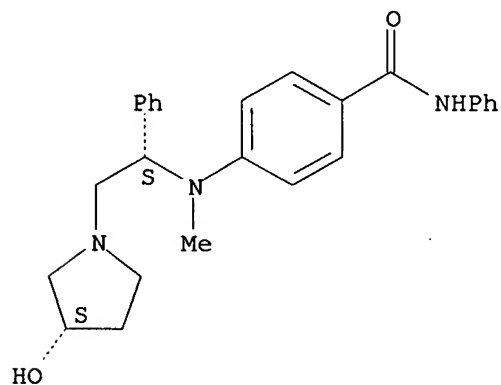
Absolute stereochemistry.



RN 204971-32-4 CAPLUS

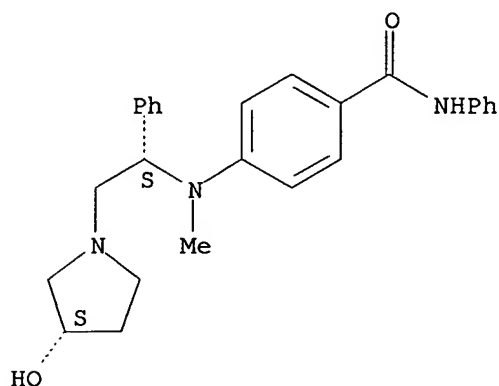
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-34-6 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

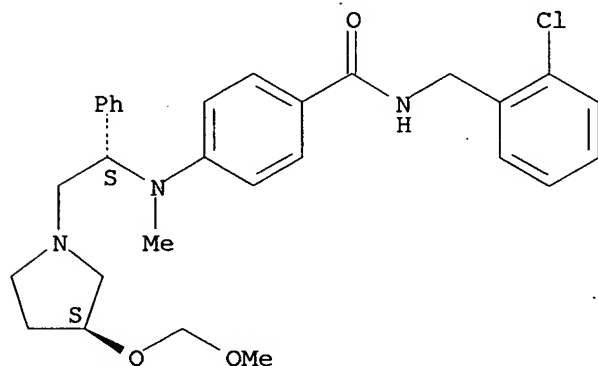
Absolute stereochemistry.



● HCl

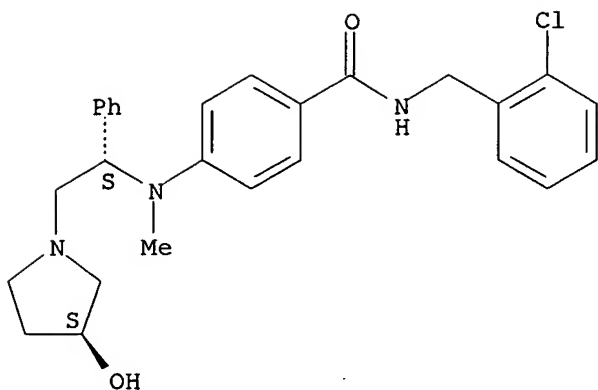
RN 204971-36-8 CAPLUS  
 CN Benzamide, N-[(2-chlorophenyl)methyl]-4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-38-0 CAPLUS  
 CN Benzamide, N-[(2-chlorophenyl)methyl]-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

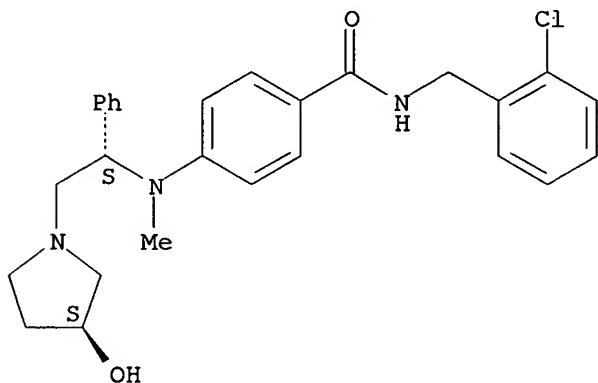
Absolute stereochemistry.



RN 204971-40-4 CAPLUS

CN Benzamide, N-[(2-chlorophenyl)methyl]-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

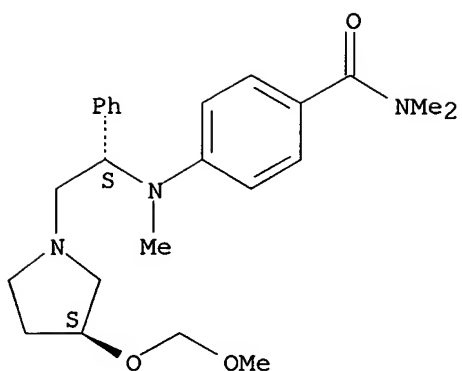


● HCl

RN 204971-42-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N,N-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

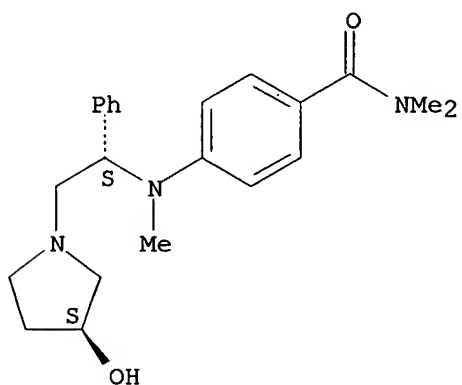
Absolute stereochemistry.



RN 204971-44-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

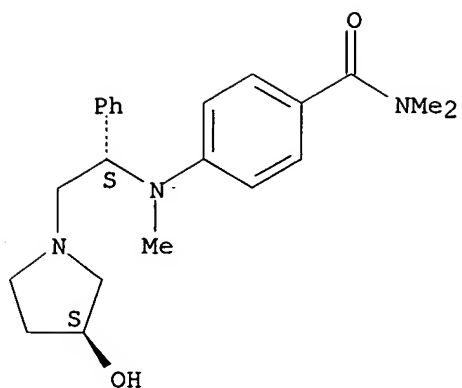
Absolute stereochemistry.



RN 204971-46-0 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N,N-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

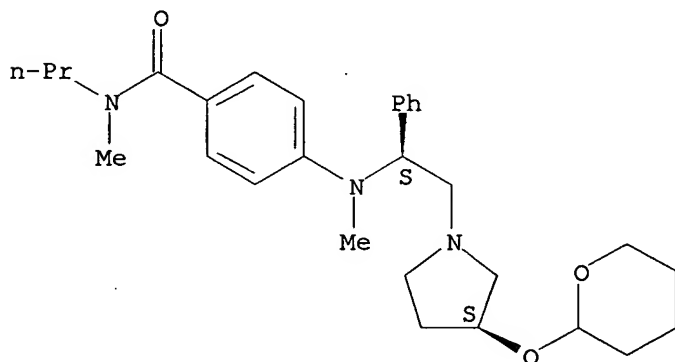


● HCl

RN 204971-48-2 CAPLUS

CN Benzamide, N-methyl-4-[methyl[(1S)-1-phenyl-2-[(3S)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-1-pyrrolidinyl]ethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

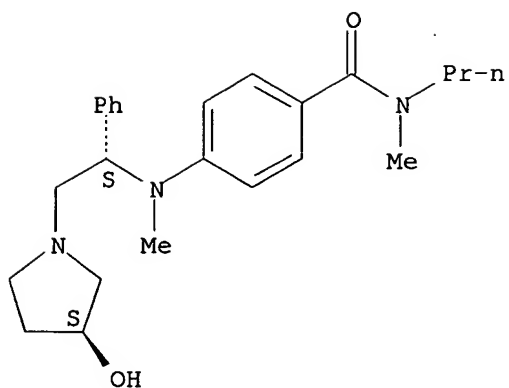
Absolute stereochemistry.



RN 204971-50-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl-N-propyl- (9CI) (CA INDEX NAME)

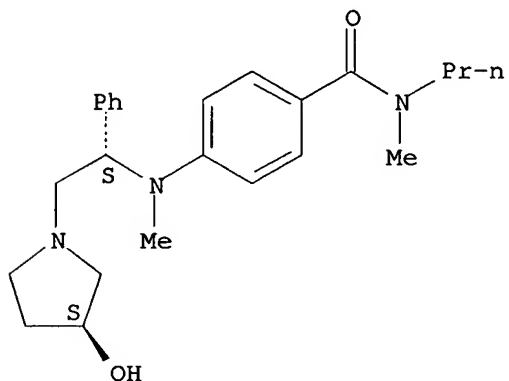
Absolute stereochemistry.



RN 204971-52-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

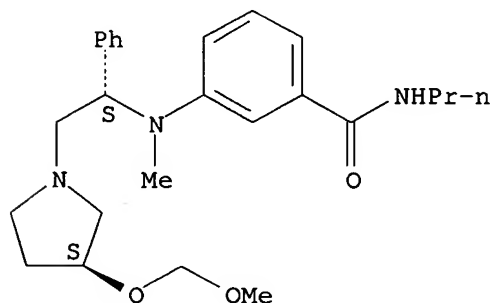


● HCl

RN 204971-54-0 CAPLUS

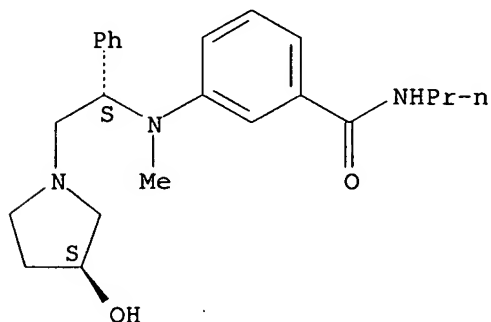
CN Benzamide, 3-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



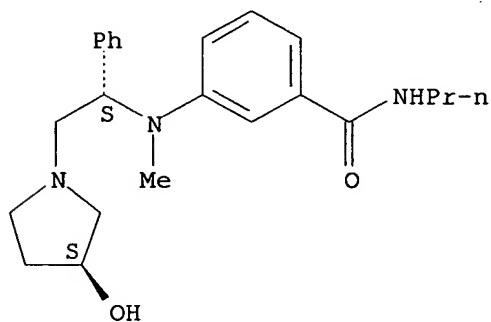
RN 204971-56-2 CAPLUS  
CN Benzamide, 3-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-58-4 CAPLUS  
CN Benzamide, 3-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

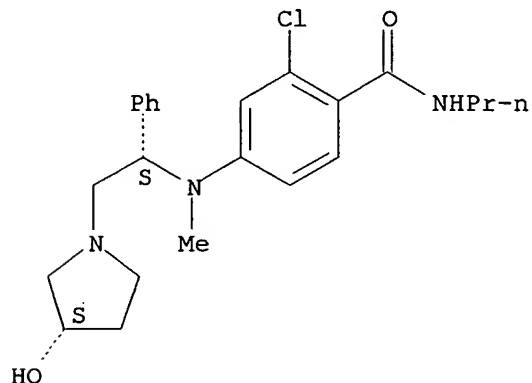
Absolute stereochemistry.



● HCl

RN 204971-61-9 CAPLUS  
CN Benzamide, 2-chloro-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

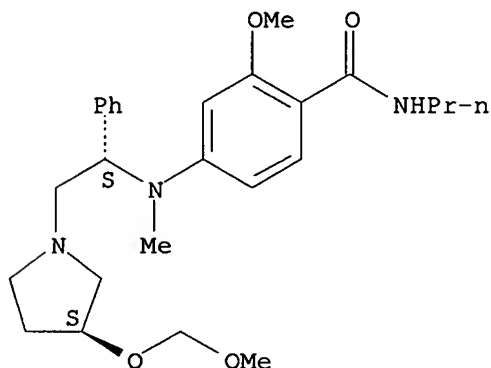




RN 204971-62-0 CAPLUS

CN Benzamide, 2-methoxy-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

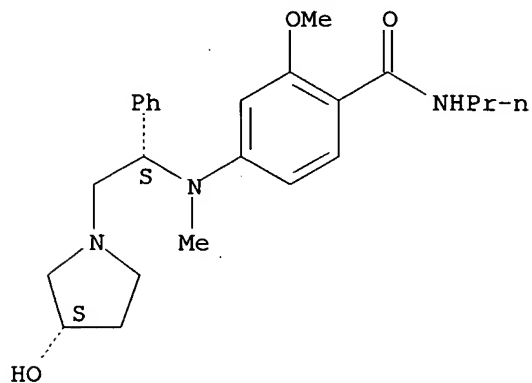
Absolute stereochemistry.



RN 204971-64-2 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-2-methoxy-N-propyl- (9CI) (CA INDEX NAME)

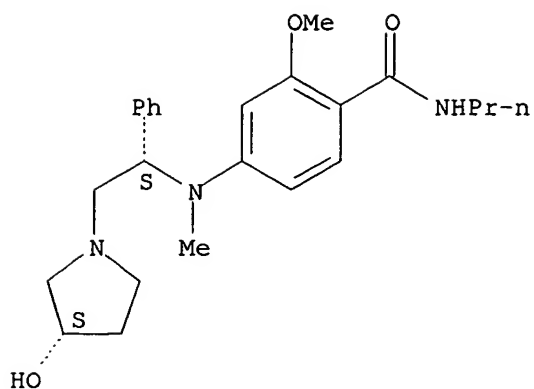
Absolute stereochemistry.



RN 204971-66-4 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-2-methoxy-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

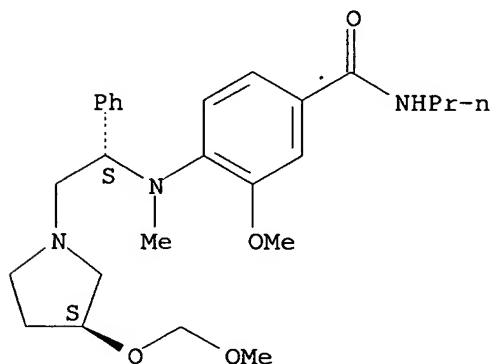


● HCl

RN 204971-67-5 CAPLUS

CN Benzamide, 3-methoxy-4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

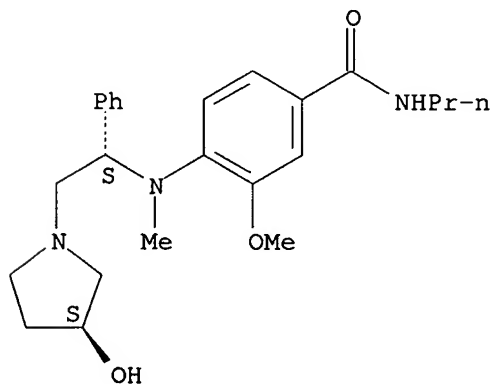
Absolute stereochemistry.



RN 204971-68-6 CAPLUS

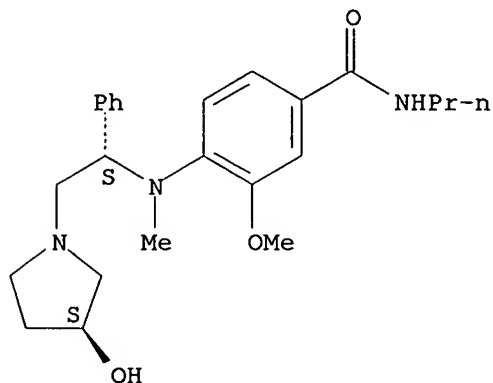
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-3-methoxy-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-69-7 CAPLUS  
CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-3-methoxy-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

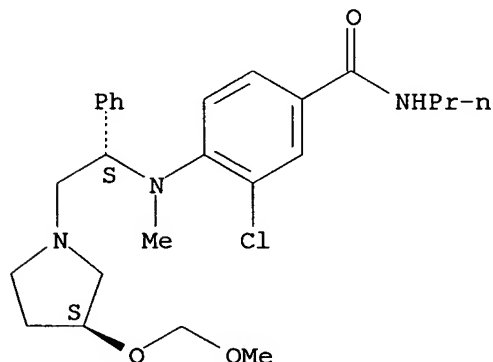
Absolute stereochemistry.



● HCl

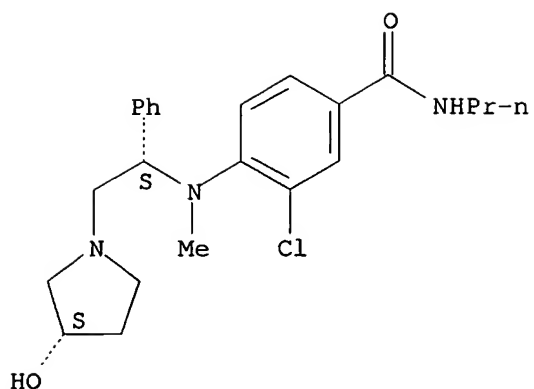
RN 204971-70-0 CAPLUS  
CN Benzamide, 3-chloro-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-71-1 CAPLUS  
CN Benzamide, 3-chloro-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

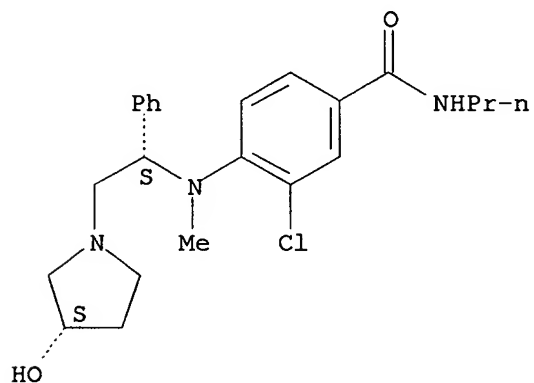


RN 204971-72-2 CAPLUS  
 CN Benzamide, 3-chloro-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204971-71-1  
 CMF C23 H30 Cl N3 O2

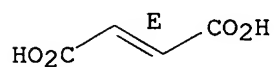
Absolute stereochemistry.



CM 2

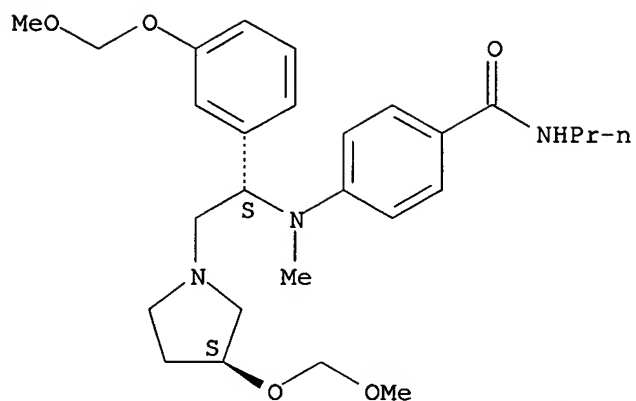
CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



RN 204971-76-6 CAPLUS  
 CN Benzamide, 4-[[ (1S)-1-[3-(methoxymethoxy)phenyl]-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

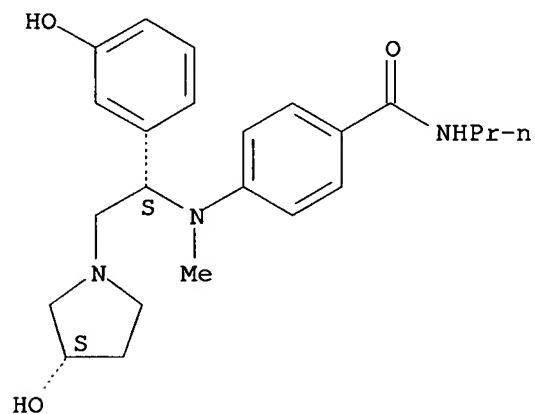
Absolute stereochemistry.



RN 204971-77-7 CAPLUS

CN Benzamide, 4-[[[(1S)-1-(3-hydroxyphenyl)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

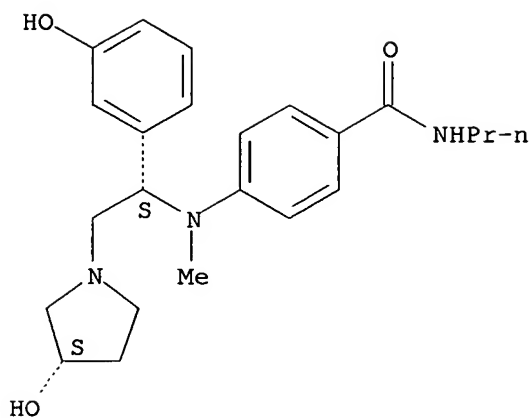
Absolute stereochemistry.



RN 204971-78-8 CAPLUS

CN Benzamide, 4-[[[(1S)-1-(3-hydroxyphenyl)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]ethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

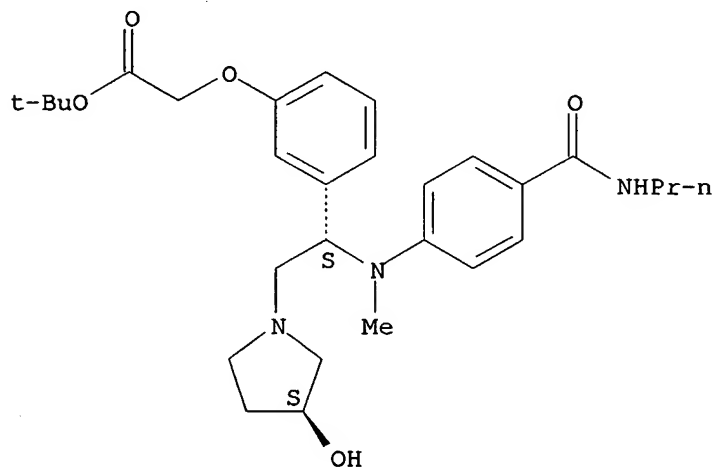


● HCl

RN 204971-79-9 CAPLUS

CN Acetic acid, [3-[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

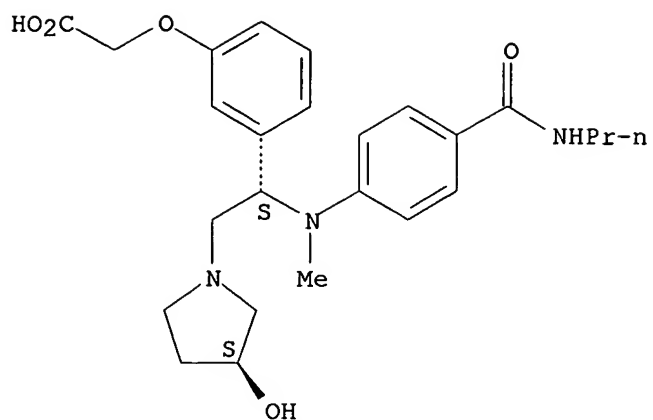
Absolute stereochemistry.



RN 204971-80-2 CAPLUS

CN Acetic acid, [3-[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]- (9CI) (CA INDEX NAME)

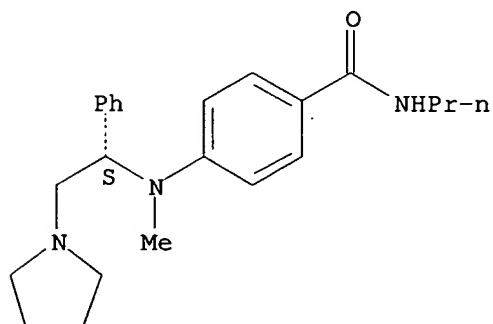
Absolute stereochemistry.



RN 204971-82-4 CAPLUS

CN Benzamide, 4-[methyl[(1S)-1-phenyl-2-(1-pyrrolidinyl)ethyl]amino]-N-propyl-  
(9CI) (CA INDEX NAME)

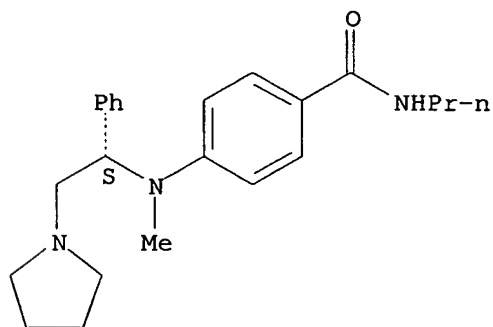
Absolute stereochemistry.



RN 204971-83-5 CAPLUS

CN Benzamide, 4-[methyl[(1S)-1-phenyl-2-(1-pyrrolidinyl)ethyl]amino]-N-propyl-  
, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



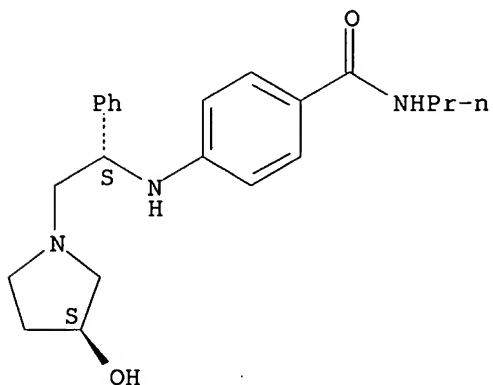
● HCl

RN 204971-89-1 CAPLUS

CN Benzamide, 4-[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]amino]-

N-propyl- (9CI) (CA INDEX NAME)

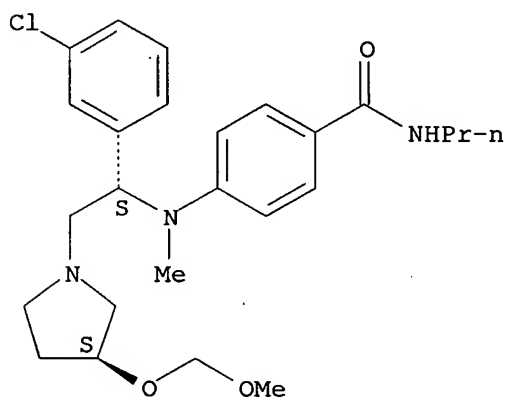
Absolute stereochemistry.



RN 204971-90-4 CAPLUS

CN Benzamide, 4-[[[(1S)-1-(3-chlorophenyl)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]ethyl]methylanilino]-N-propyl- (9CI) (CA INDEX NAME)

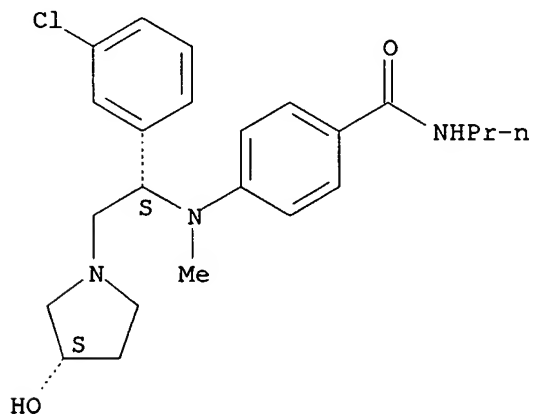
Absolute stereochemistry.



RN 204971-91-5 CAPLUS

CN Benzamide, 4-[[[(1S)-1-(3-chlorophenyl)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]ethyl]methylanilino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



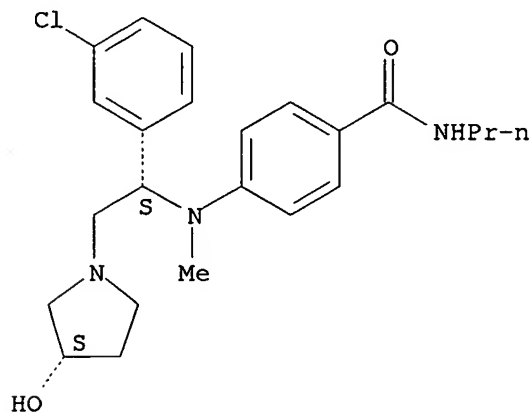


RN 204971-92-6 CAPLUS  
CN Benzamide, 4-[[[(1S)-1-(3-chlorophenyl)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]ethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1)  
(salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204971-91-5  
CMF C23 H30 Cl N3 O2

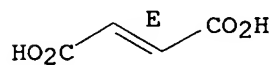
Absolute stereochemistry.



CM 2

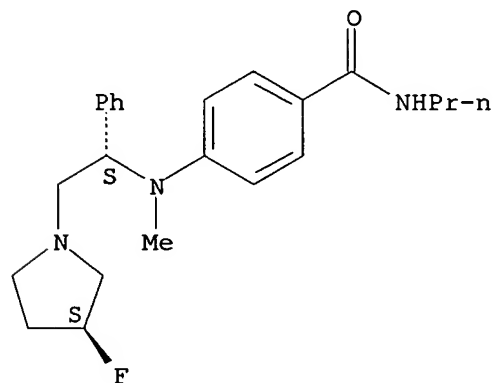
CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.



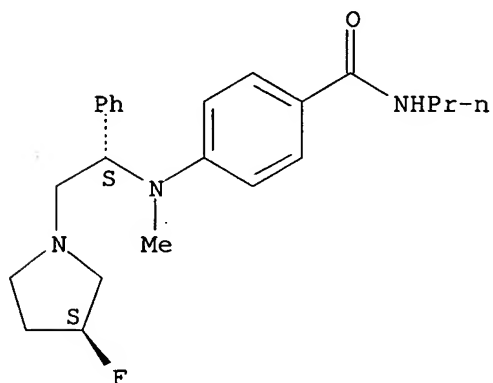
RN 204971-93-7 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-94-8 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

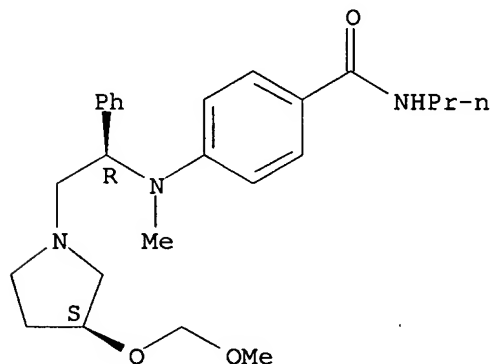
Absolute stereochemistry.



● HCl

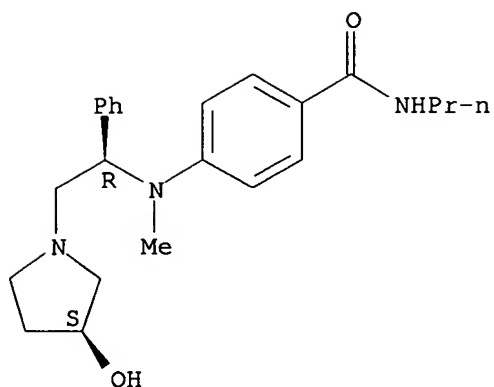
RN 204971-95-9 CAPLUS  
CN Benzamide, 4-[[[(1R)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-96-0 CAPLUS  
CN Benzamide, 4-[[[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

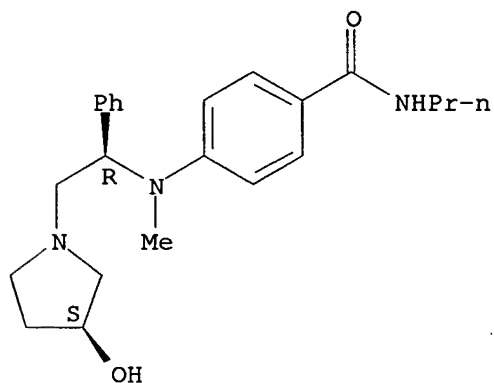
Absolute stereochemistry.



RN 204971-97-1 CAPLUS

CN Benzamide, 4-[[[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

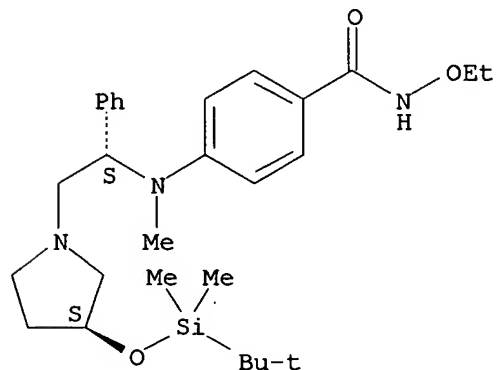


● HCl

RN 204972-01-0 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-ethoxy- (9CI) (CA INDEX NAME)

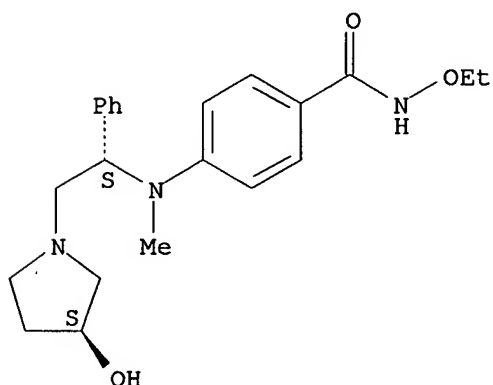
Absolute stereochemistry.



RN 204972-02-1 CAPLUS

CN Benzamide, N-ethoxy-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

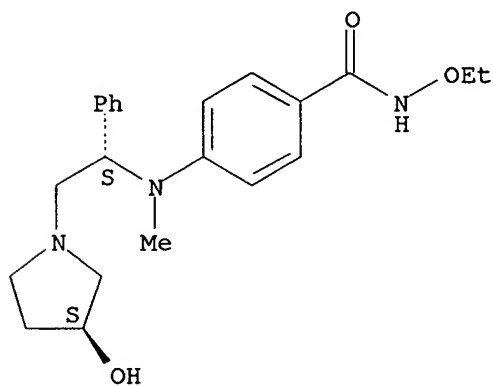
Absolute stereochemistry.



RN 204972-03-2 CAPLUS

CN Benzamide, N-ethoxy-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

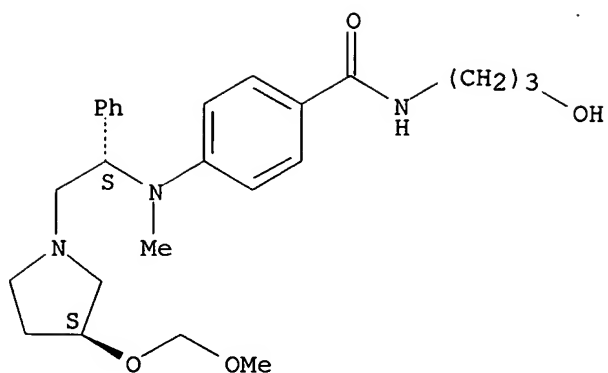


● HCl

RN 204972-07-6 CAPLUS

CN Benzamide, N-(3-hydroxypropyl)-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

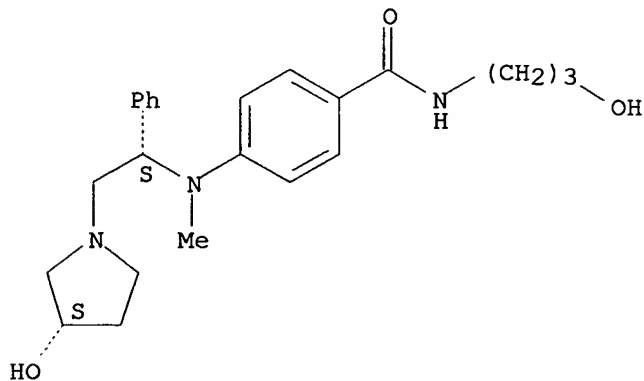
Absolute stereochemistry.



RN 204972-08-7 CAPLUS

CN Benzamide, N-(3-hydroxypropyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

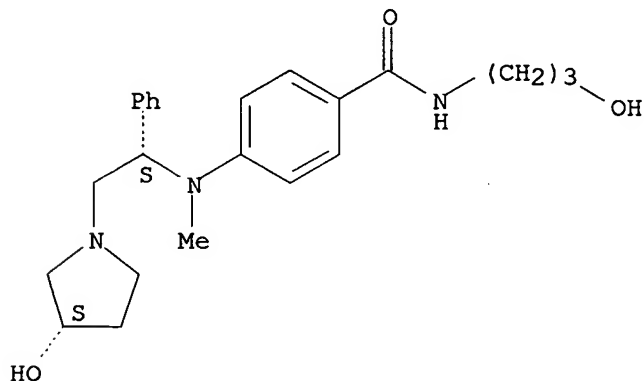
Absolute stereochemistry.



RN 204972-09-8 CAPLUS

CN Benzamide, N-(3-hydroxypropyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

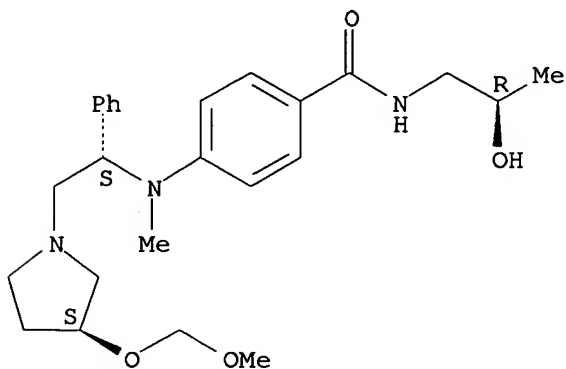


● HCl

RN 204972-10-1 CAPLUS

CN Benzamide, N-[(2R)-2-hydroxypropyl]-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

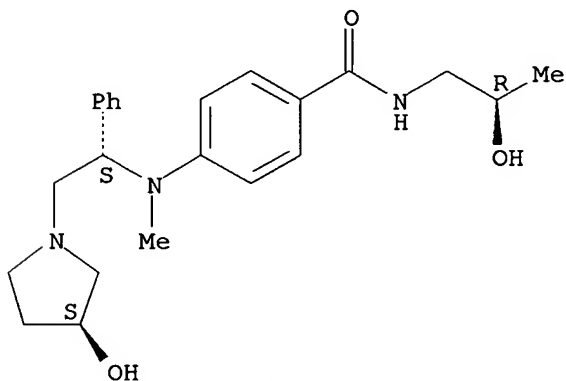
Absolute stereochemistry.



RN 204972-11-2 CAPLUS

CN Benzamide, N-[(2R)-2-hydroxypropyl]-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

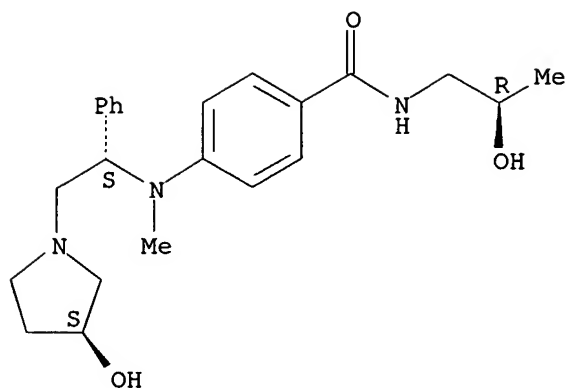
Absolute stereochemistry.



RN 204972-12-3 CAPLUS

CN Benzamide, N-[(2R)-2-hydroxypropyl]-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

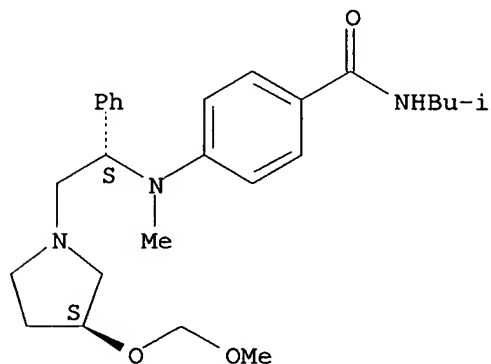


● HCl

RN 204972-13-4 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

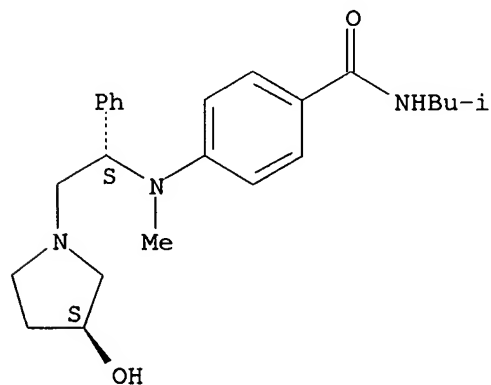
Absolute stereochemistry.



RN 204972-14-5 CAPLUS

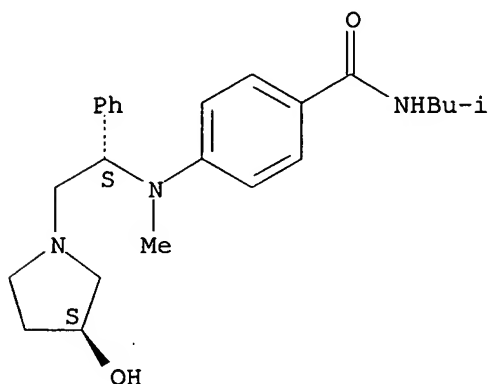
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-15-6 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2-methylpropyl)-, monohydrochloride (9CI) (CA INDEX NAME)

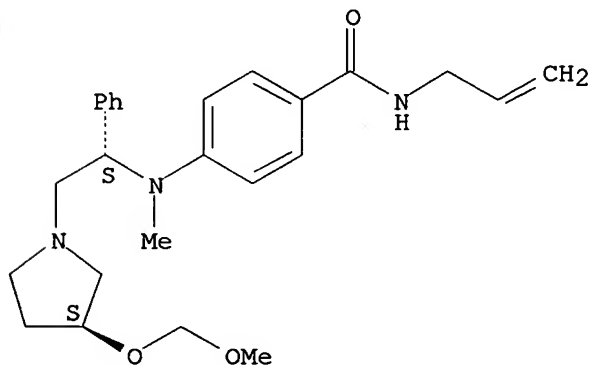
Absolute stereochemistry.



● HCl

RN 204972-16-7 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propenyl- (9CI) (CA INDEX NAME)

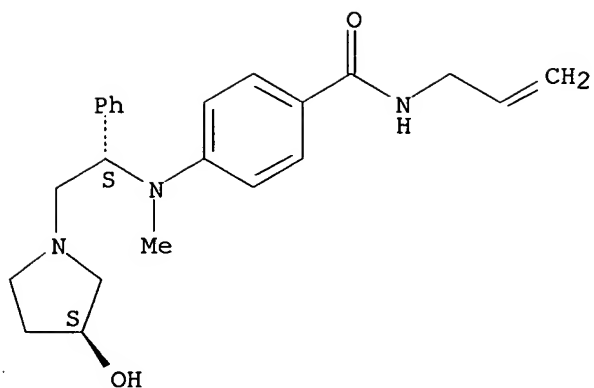
Absolute stereochemistry.



RN 204972-17-8 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

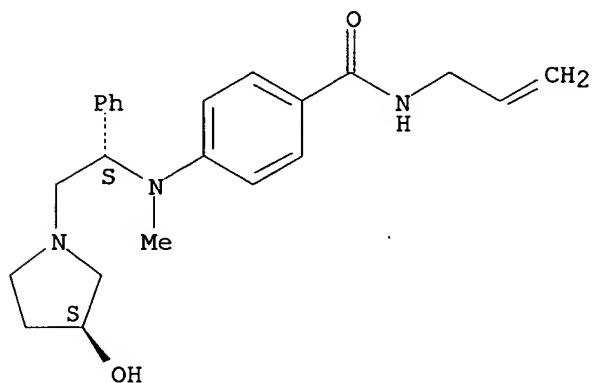




RN 204972-18-9 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propenyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

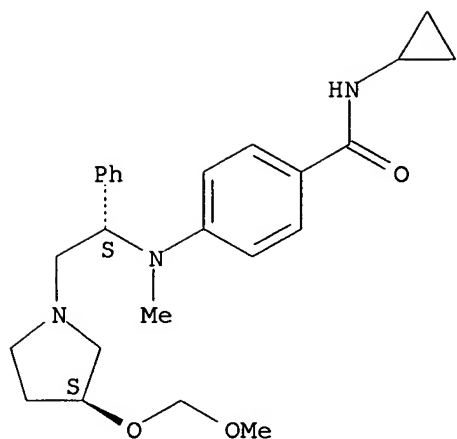


● HCl

RN 204972-19-0 CAPLUS

CN Benzamide, N-cyclopropyl-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

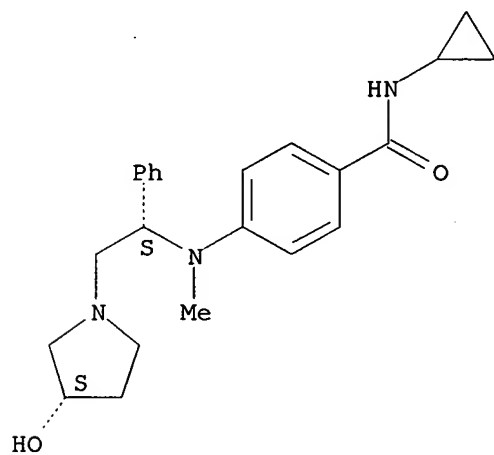
Absolute stereochemistry.



RN 204972-20-3 CAPLUS

CN Benzamide, N-cyclopropyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

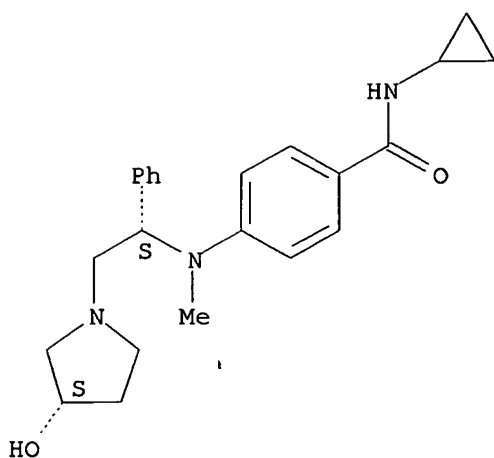
Absolute stereochemistry.



RN 204972-21-4 CAPLUS

CN Benzamide, N-cyclopropyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

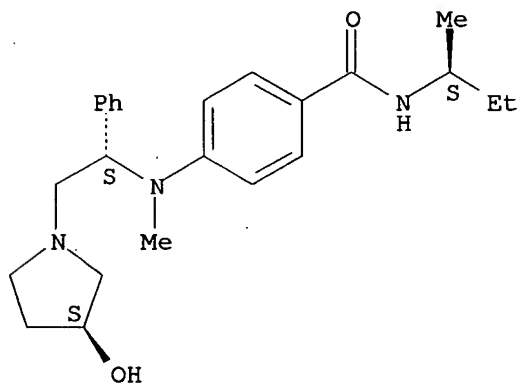
Absolute stereochemistry.



● HCl

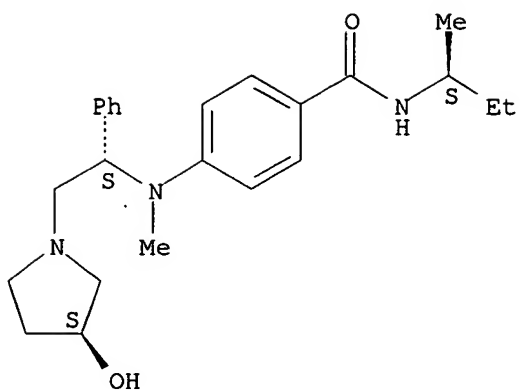
RN 204972-22-5 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1S)-1-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-23-6 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1S)-1-methylpropyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

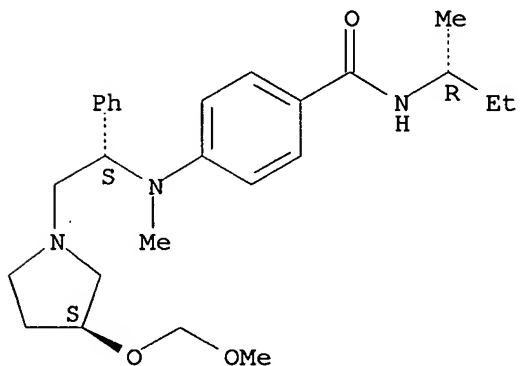


● HCl

RN 204972-24-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1R)-1-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-25-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1R)-1-methylpropyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1R)-1-methylpropyl]- (9CI) (CA INDEX NAME)

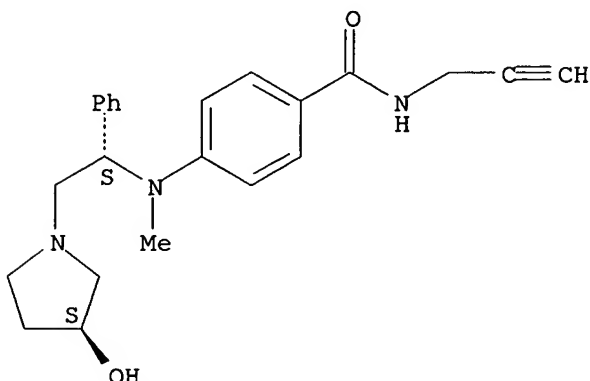
Chemical structure of a substituted pyrrolidine derivative. The pyrrolidine ring has a hydroxyl group (OH) at the 2-position. The nitrogen atom is substituted with a 1-phenylethyl group (Ph-CH<sub>2</sub>-CH(S)-) and a methyl group (Me). The 1-phenylethyl group is further substituted with a benzoyl group (C(=O)-NH-CH(Me)-Et) at the 1-position.

CN    Benzanide, 4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propynyl- (9CI)    (CA INDEX NAME)

COCOC[C@H]1S[C@@H](CN(C)C(=O)c2ccc(cc2)N(C)C[C@H](CN3CCCC3)C4=CC=CC=C4)C1

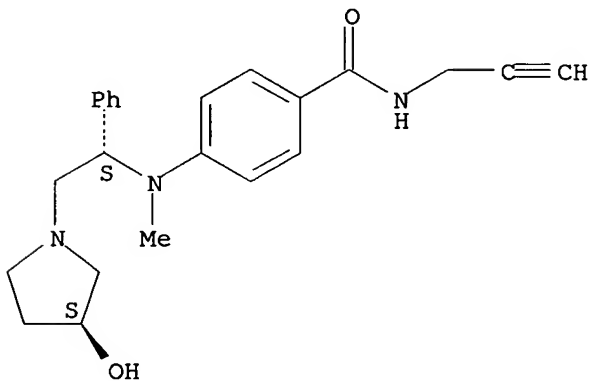
RN 204972-28-1 CAPLUS  
CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-29-2 CAPLUS  
CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propynyl-, monohydrochloride (9CI) (CA INDEX NAME)

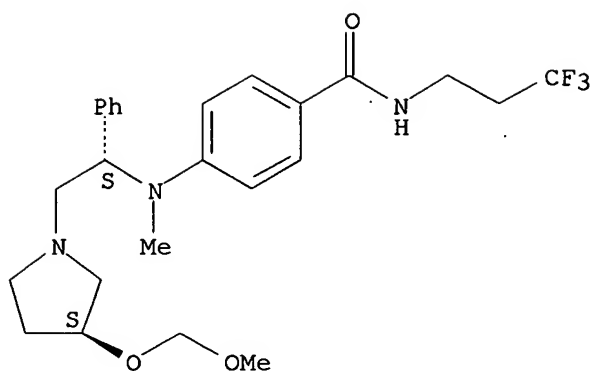
Absolute stereochemistry.



● HCl

RN 204972-30-5 CAPLUS  
CN Benzamide, 4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

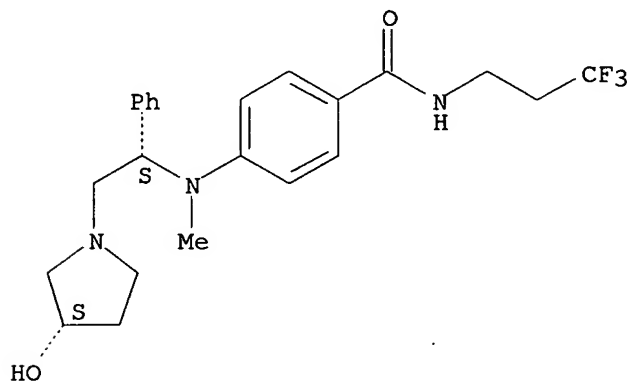
Absolute stereochemistry.



RN 204972-31-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

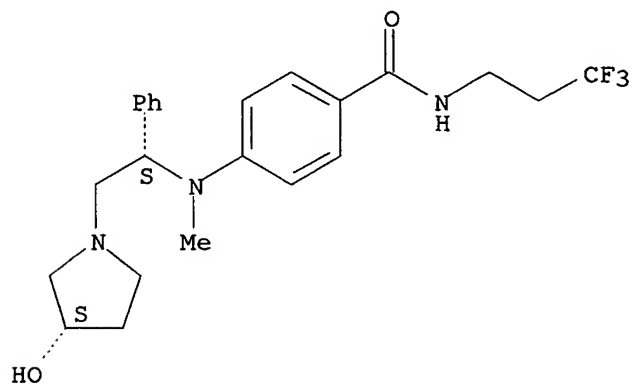
Absolute stereochemistry.



RN 204972-32-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(3,3,3-trifluoropropyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

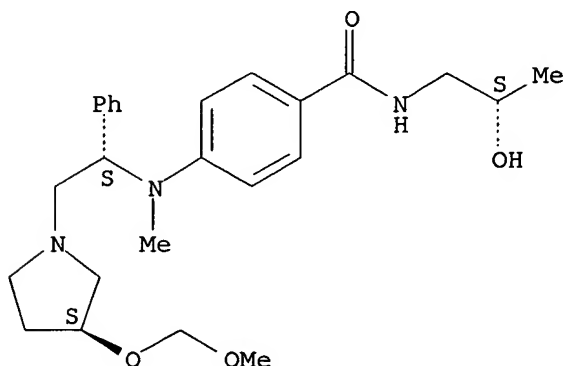


● HCl

RN 204972-33-8 CAPLUS

CN Benzamide, N-[(2S)-2-hydroxypropyl]-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

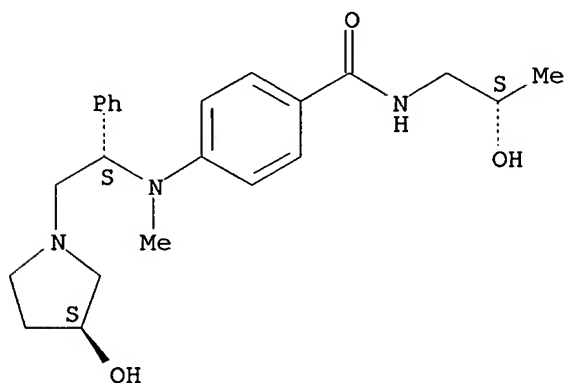
Absolute stereochemistry.



RN 204972-34-9 CAPLUS

CN Benzamide, N-[(2S)-2-hydroxypropyl]-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-35-0 CAPLUS

CN Benzamide, N-[(2S)-2-hydroxypropyl]-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

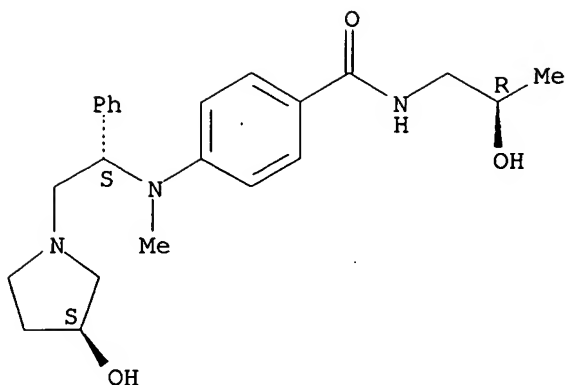
CM 1

CRN 204972-11-2

CMF C23 H31 N3 O3

Absolute stereochemistry.



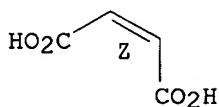


CM 2

CRN 110-16-7

CMF C4 H4 O4

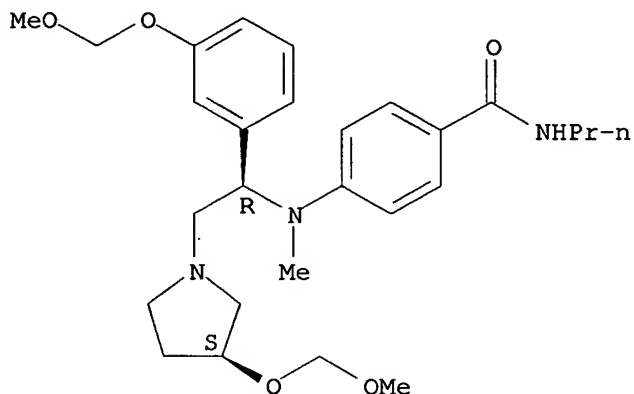
Double bond geometry as shown.



RN 204972-36-1 CAPLUS

CN Benzamide, 4-[[ (1R)-1-[3-(methoxymethoxy)phenyl]-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

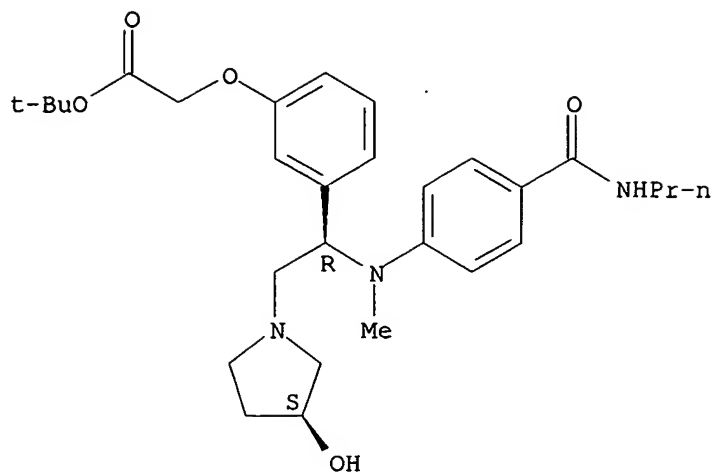
Absolute stereochemistry.



RN 204972-37-2 CAPLUS

CN Acetic acid, [3-[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

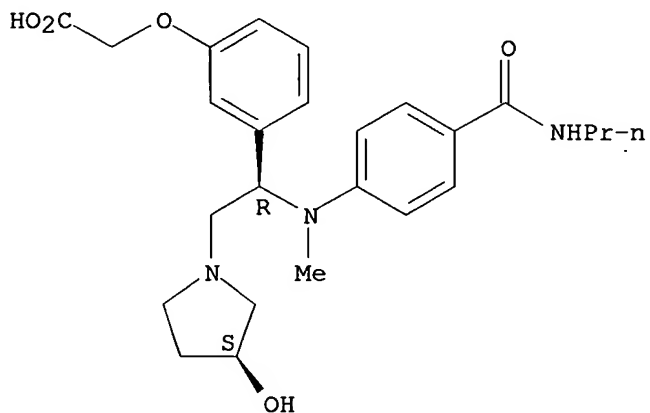
Absolute stereochemistry.



RN 204972-38-3 CAPLUS

CN Acetic acid, [3-[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]- (9CI) (CA INDEX NAME)

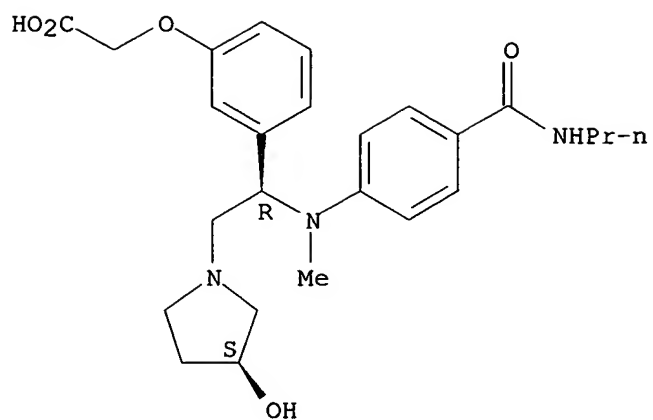
Absolute stereochemistry.



RN 204972-39-4 CAPLUS

CN Acetic acid, [3-[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

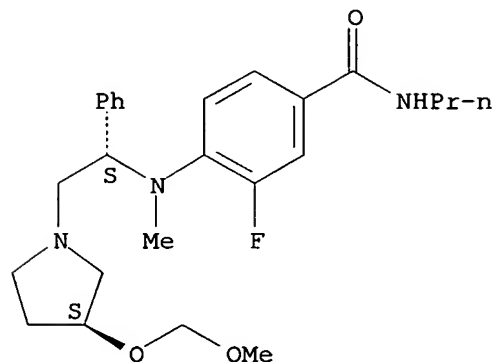


● HCl

RN 204972-40-7 CAPLUS

CN Benzamide, 3-fluoro-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

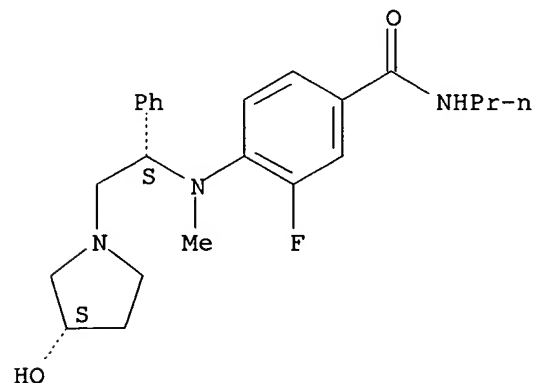
Absolute stereochemistry.



RN 204972-41-8 CAPLUS

CN Benzamide, 3-fluoro-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

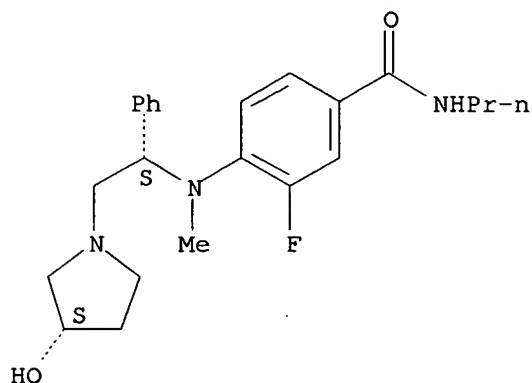


RN 204972-42-9 CAPLUS  
CN Benzamide, 3-fluoro-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2Z)-2-butenedioate (1:1) (salt) (9CI)  
(CA INDEX NAME)

CM 1

CRN 204972-41-8  
CMF C23 H30 F N3 O2

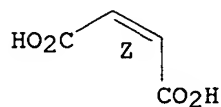
Absolute stereochemistry.



CM 2

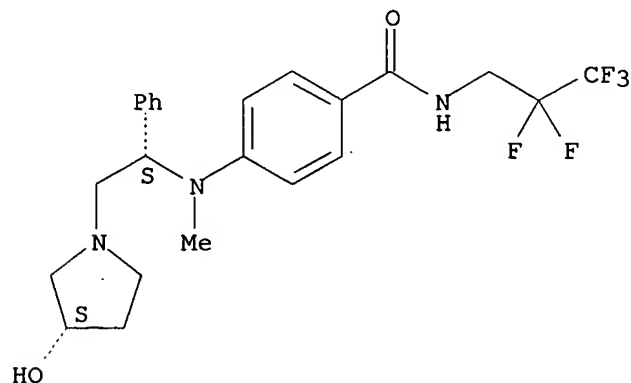
CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.



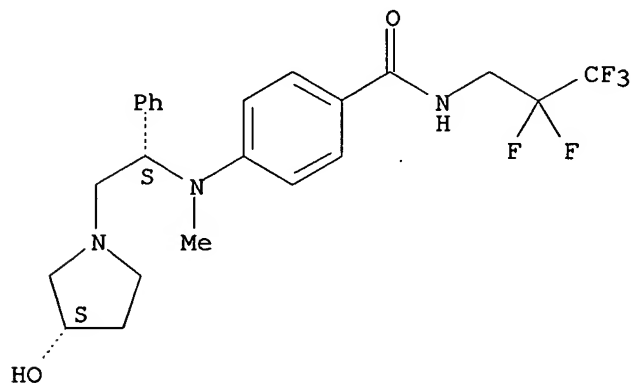
RN 204972-43-0 CAPLUS  
CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-44-1 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2,2,3,3,3-pentafluoropropyl)-, monohydrochloride (9CI) (CA INDEX NAME)

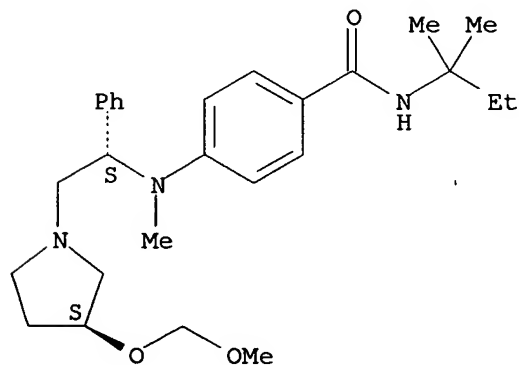
Absolute stereochemistry.



● HCl

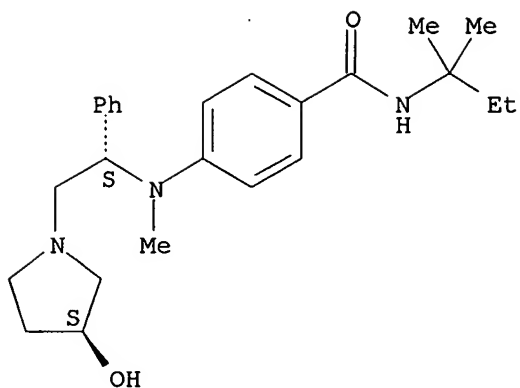
RN 204972-45-2 CAPLUS  
 CN Benzamide, N-(1,1-dimethylpropyl)-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-46-3 CAPLUS  
 CN Benzamide, N-(1,1-dimethylpropyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

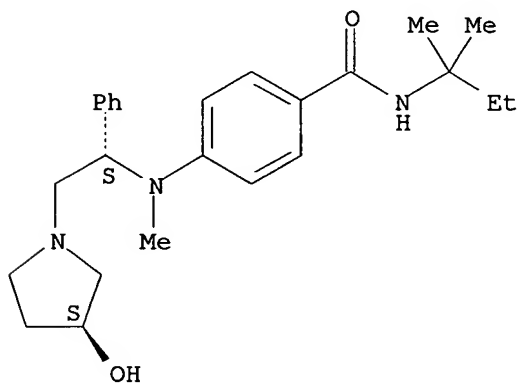
Absolute stereochemistry.



RN 204972-47-4 CAPLUS

CN Benzamide, N-(1,1-dimethylpropyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

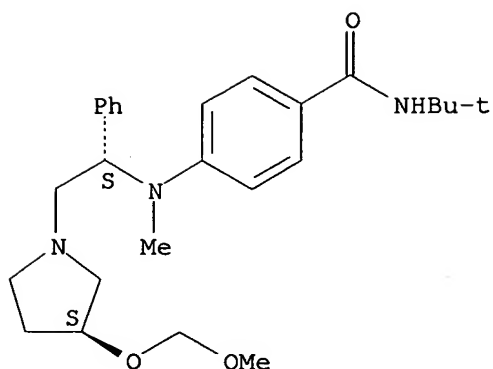


● HCl

RN 204972-48-5 CAPLUS

CN Benzamide, N-(1,1-dimethylethyl)-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

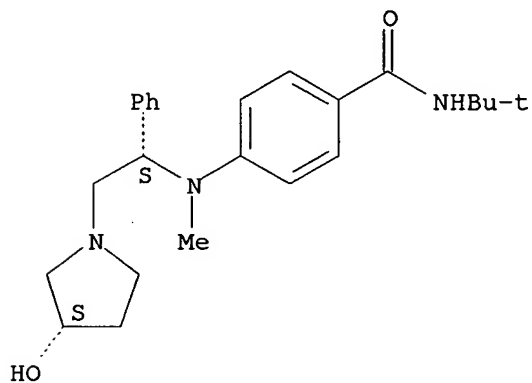
Absolute stereochemistry.



RN 204972-49-6 CAPLUS

CN Benzamide, N-(1,1-dimethylethyl)-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

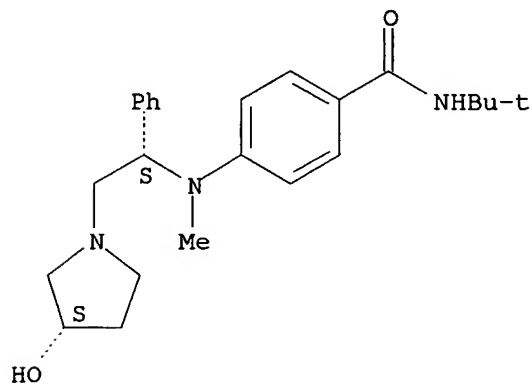
Absolute stereochemistry.



RN 204972-50-9 CAPLUS

CN Benzamide, N-(1,1-dimethylethyl)-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

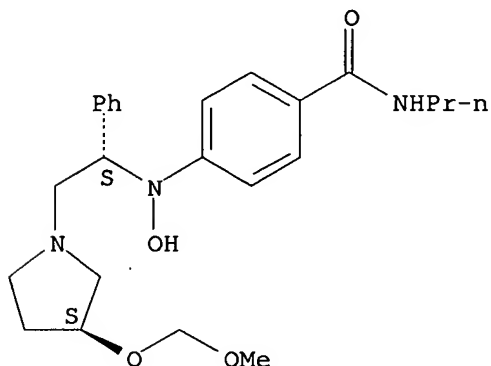


● HCl

RN 204972-53-2 CAPLUS

CN Benzamide, 4-[hydroxy[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

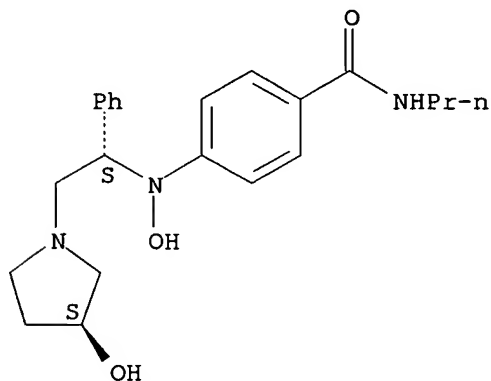
Absolute stereochemistry.



RN 204972-54-3 CAPLUS

CN Benzamide, 4-[hydroxy[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

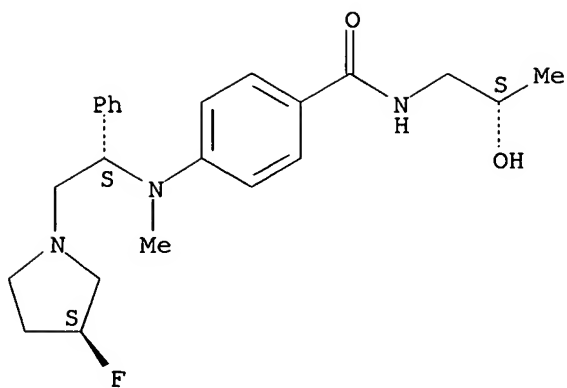


RN 204972-56-5 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2S)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



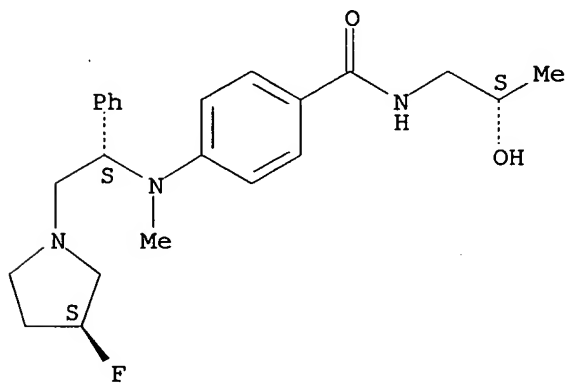


RN 204972-57-6 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2S)-2-hydroxypropyl]-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204972-56-5  
 CMF C23 H30 F N3 O2

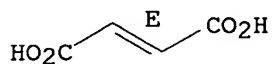
Absolute stereochemistry.



CM 2

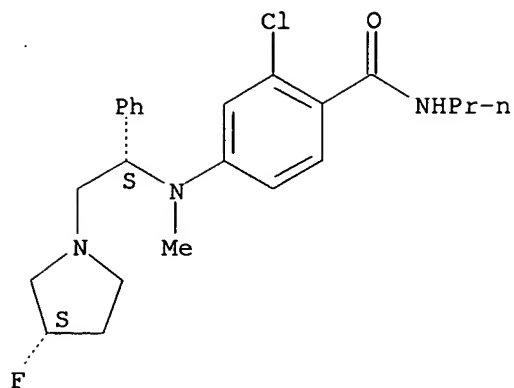
CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



RN 204972-58-7 CAPLUS  
 CN Benzamide, 2-chloro-4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

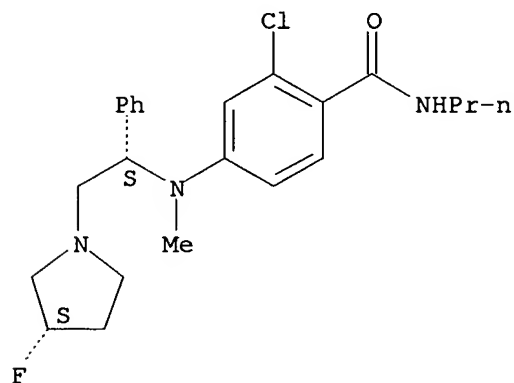


RN 204972-59-8 CAPLUS  
 CN Benzamide, 2-chloro-4-[[ (1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 204972-58-7  
 CMF C23 H29 Cl F N3 O

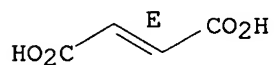
Absolute stereochemistry.



CM 2

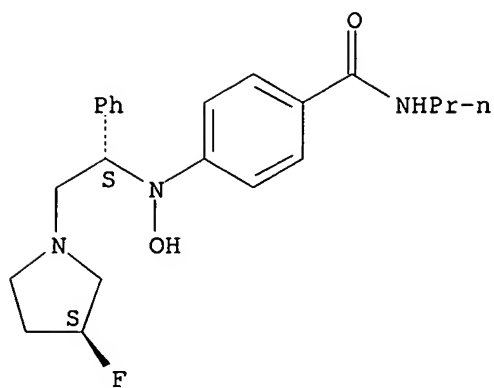
CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



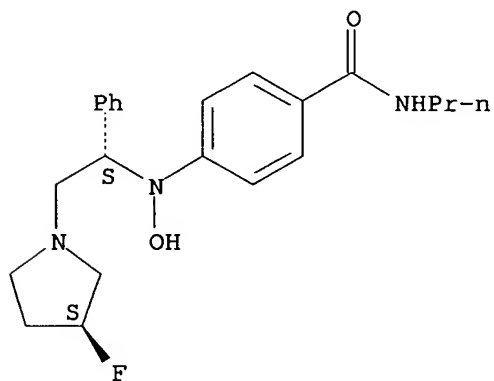
RN 204972-60-1 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]hydroxyamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-61-2 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]hydroxyamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

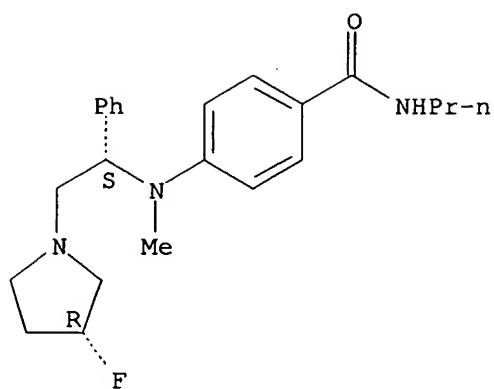
Absolute stereochemistry.



● HCl

RN 204972-66-7 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3R)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methyamino]-N-propyl- (9CI) (CA INDEX NAME)

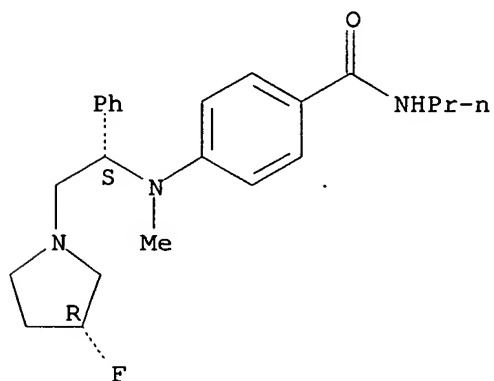
Absolute stereochemistry.



RN 204972-67-8 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3R)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

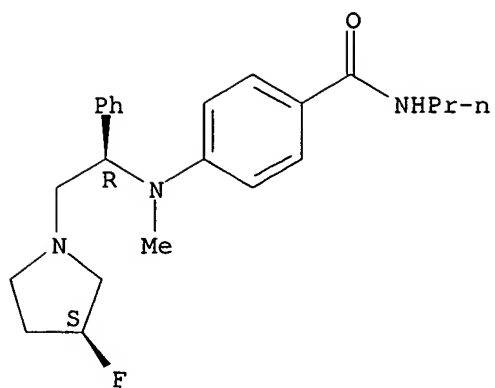


● HCl

RN 204972-68-9 CAPLUS

CN Benzamide, 4-[[ (1R)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

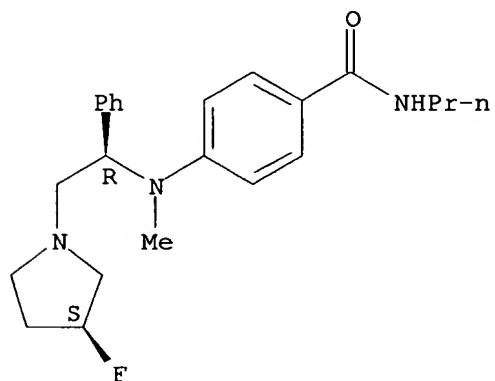
Absolute stereochemistry.



RN 204972-69-0 CAPLUS

CN Benzamide, 4-[[[(1R)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methanamine]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

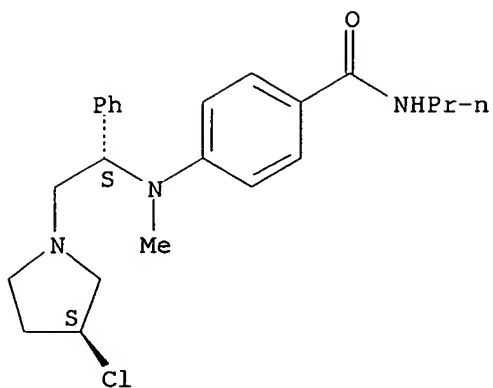


● HCl

RN 204972-70-3 CAPLUS

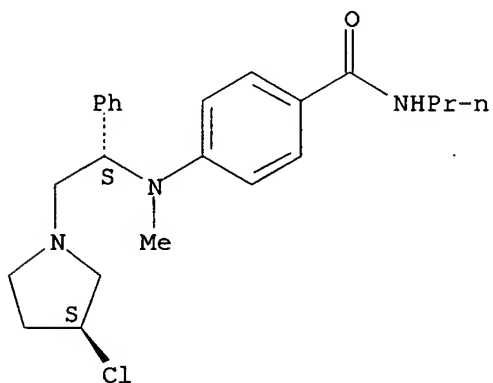
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methanamine]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-71-4 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

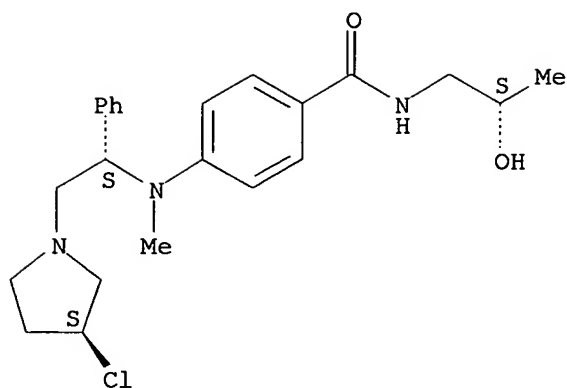
Absolute stereochemistry.



● HCl

RN 204972-72-5 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2S)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

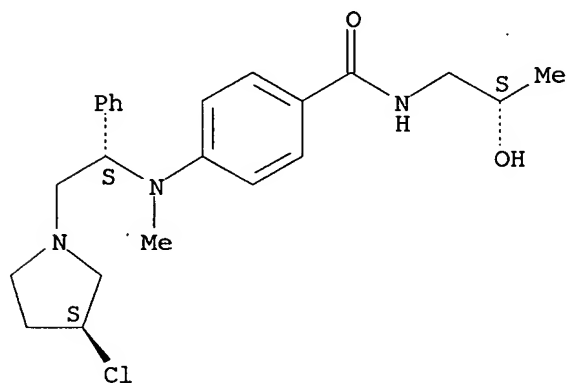
Absolute stereochemistry.



RN 204972-73-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2S)-2-hydroxypropyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

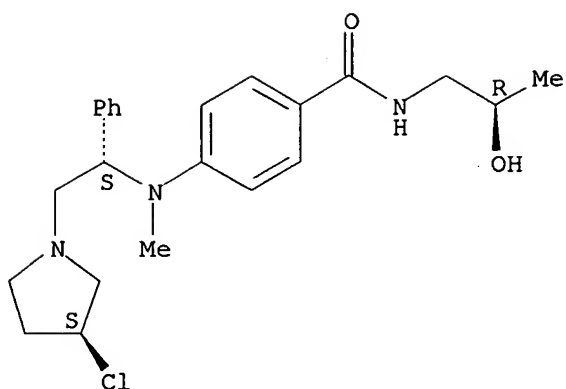


● HCl

RN 204972-74-7 CAPLUS

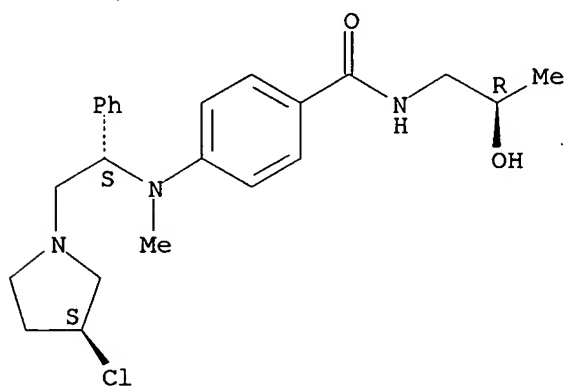
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2R)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-75-8 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2R)-2-hydroxypropyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

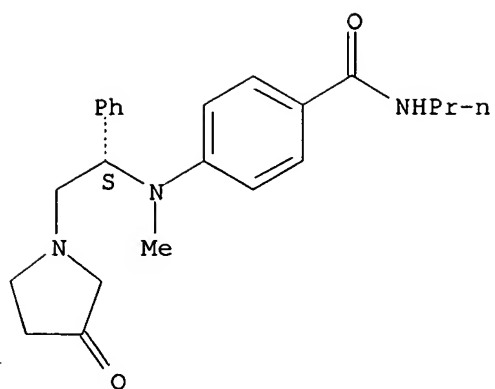


● HCl

RN 204972-76-9 CAPLUS  
 CN Benzamide, 4-[methyl[(1S)-2-(3-oxo-1-pyrrolidinyl)-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

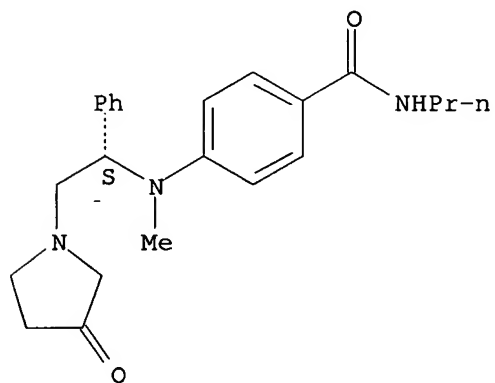




RN 204972-77-0 CAPLUS

CN Benzamide, 4-[methyl[(1S)-2-(3-oxo-1-pyrrolidinyl)-1-phenylethyl]amino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

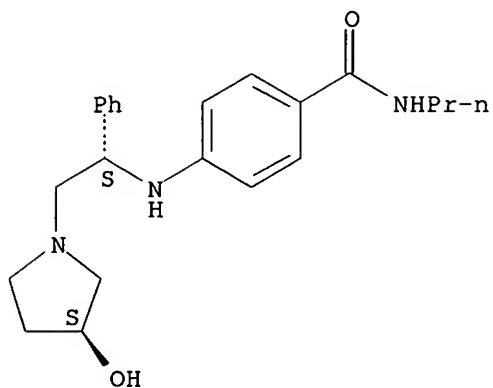


● HCl

RN 204973-49-9 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

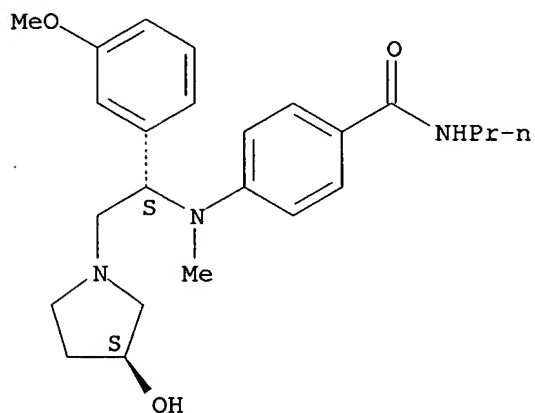


● HCl

RN 204973-55-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-(3-methoxyphenyl)ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

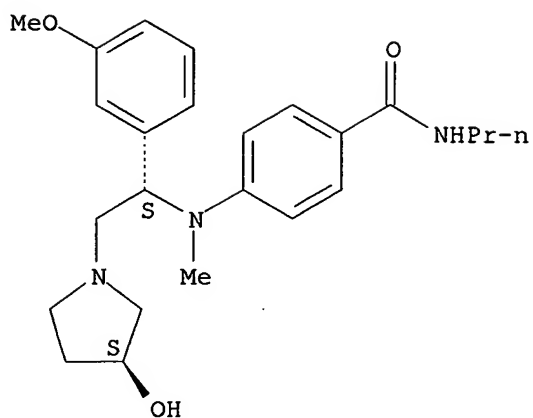
Absolute stereochemistry.



RN 204973-56-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-(3-methoxyphenyl)ethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

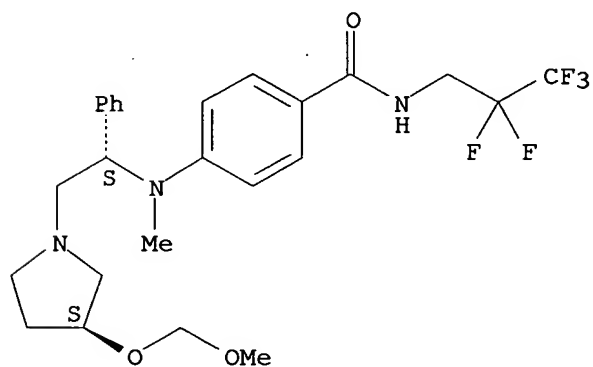


● HCl

RN 204995-07-3 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

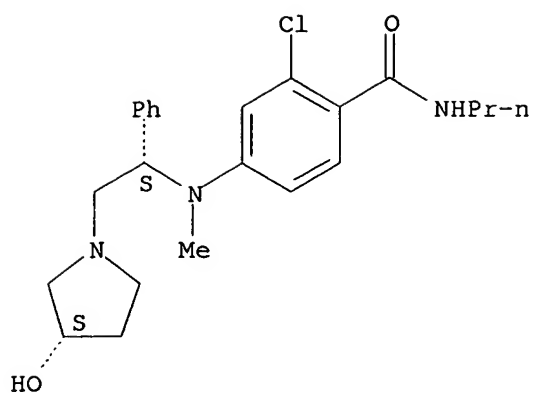
Absolute stereochemistry.



RN 329365-40-4 CAPLUS

CN Benzamide, 2-chloro-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

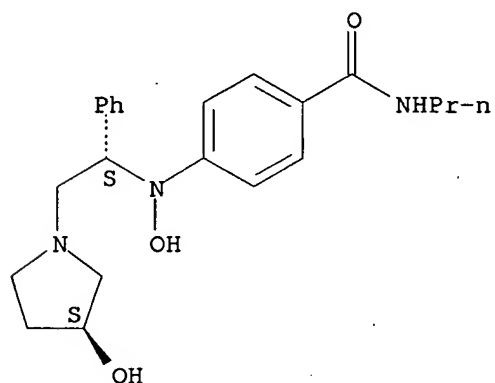
Absolute stereochemistry.



● HCl

RN 329365-41-5 CAPLUS  
 CN Benzamide, 4-[hydroxy[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

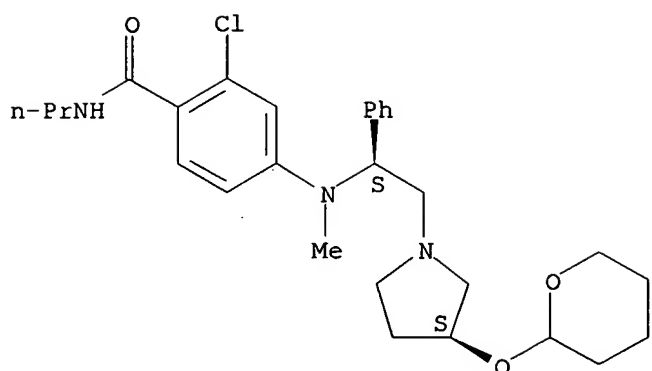
Absolute stereochemistry.



● HCl

RN 329365-43-7 CAPLUS  
 CN Benzamide, 2-chloro-4-[methyl[(1S)-1-phenyl-2-[(3S)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-1-pyrrolidinyl]ethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

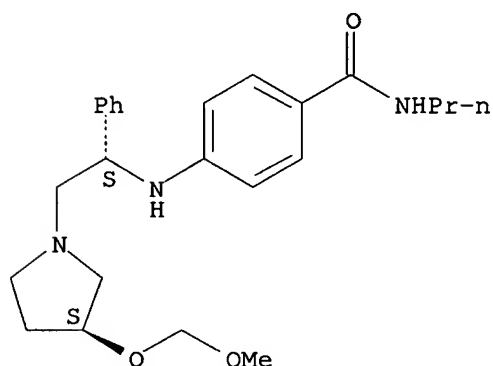
Absolute stereochemistry.



RN 329365-44-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl]- (9CI) (CA INDEX NAME)

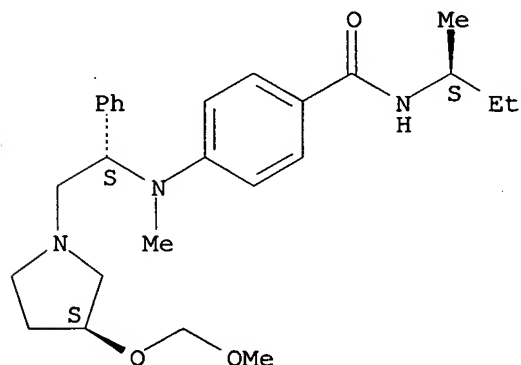
Absolute stereochemistry.



RN 329365-45-9 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(1-methylpropyl)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

6

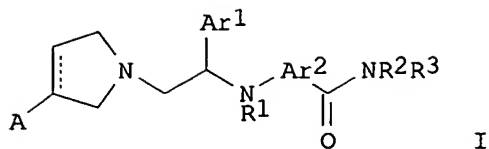
THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:199673 CAPLUS

DOCUMENT NUMBER: 128:243949  
 TITLE: Preparation of pyrrolidinyl- and pyrrolinylethylamines as kappa agonists.  
 INVENTOR(S): Ito, Fumitaka; Kondo, Hiroshi  
 PATENT ASSIGNEE(S): Pfizer Inc., USA; Pfizer Pharmaceuticals Inc.  
 SOURCE: PCT Int. Appl., 129 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9812177	A1	19980326	WO 1997-IB1021	19970821
W: AU, BG, BR, CA, CN, CZ, HU, IL, IS, JP, KR, LK, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
TW 432047	B	20010501	TW 1997-86111948	19970820
AU 9737812	A1	19980414	AU 1997-37812	19970821
AU 719895	B2	20000518		
EP 934264	A1	19990811	EP 1997-934676	19970821
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LV, FI, RO				
BR 9711506	A	19990824	BR 1997-11506	19970821
CN 1237962	A	19991208	CN 1997-199817	19970821
JP 2000516634	T2	20001212	JP 1998-514433	19970821
JP 3195368	B2	20010806		
JP 2001316344	A2	20011113	JP 2001-92342	19970821
AT 249433	E	20030915	AT 1997-934676	19970821
CA 2266006	C	20031104	CA 1997-2266006	19970821
CA 2266006	AA	19980326		
PT 934264	T	20040130	PT 1997-934676	19970821
ES 2205248	T3	20040501	ES 1997-934676	19970821
AP 1016	A	20011008	AP 1997-1082	19970911
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ZA 9708358	A	19990317	ZA 1997-8358	19970917
BG 64194	B1	20040430	BG 1999-103239	19990311
US 6201007	B1	20010313	US 1999-254805	19990312
NO 9901294	A	19990317	NO 1999-1294	19990317
KR 2000036225	A	20000626	KR 1999-702287	19990317
US 2001008890	A1	20010719	US 2001-770515	20010126
US 6310061	B2	20011030		
US 2001009921	A1	20010726	US 2001-770513	20010126
US 6313302	B2	20011106		
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US 6294569	B2	20010925		
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US 6307061	B2	20011023		
US 2001020024	A1	20010906	US 2001-771030	20010126
US 6294557	B2	20010925		
US 6303602	B1	20011016	US 2001-770512	20010126
PRIORITY APPLN. INFO.:				
				WO 1996-IB957 A 19960918
				JP 1998-514433 A3 19970821
				WO 1997-IB1021 W 19970821
				US 1999-254805 A3 19990312
OTHER SOURCE(S): MARPAT 128:243949				
GI				



AB Title compds. [I; A = null, H, halo, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, etc.; dotted line = optional double bond; Ar1 = (substituted) Ph; Ar2 = (substituted) Ph, naphthyl, pyridyl, thienyl, furyl, pyrrolyl, pyrimidinyl; R1 = H, OH, alkyl, alkoxy, etc.; R2, R3 = H, OH, (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, alkoxy, Ph, phenylalkyl, etc.; R2R3N = (substituted) pyrrolidinyl, piperidinyl, morpholinyl], were prepared Thus, 2-[3(S)-methoxymethoxypyrrolidin-1-yl]-1(RS)-phenylethanol (preparation given) and Et3N in CH2Cl2 were treated with MeSO2Cl at 0° to give a residue which was refluxed with Me 4-methylaminobenzoate in EtOH to give 62.5% Me 4-[N-[2-[3(S)-methoxymethoxypyrrolidin-1-yl]-1(S)-phenylethyl]-N-methylamino]benzoate. This was saponified with 4N NaOH in MeOH (100%) and the resulting acid was stirred with PrNH2 and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride in CH2Cl2 to give 72% 4-[N-[2-[3(S)-methoxymethoxypyrrolidin-1-yl]-1(S)-phenylethyl]-N-methylamino]-N'-propylbenzamide. Some I inhibited acute pain in rats with ED50 <10 mg/kg orally.

IT 204970-95-6P 204970-97-8P 204970-99-0P  
 204971-01-7P 204971-03-9P 204971-05-1P  
 204971-07-3P 204971-09-5P 204971-11-9P  
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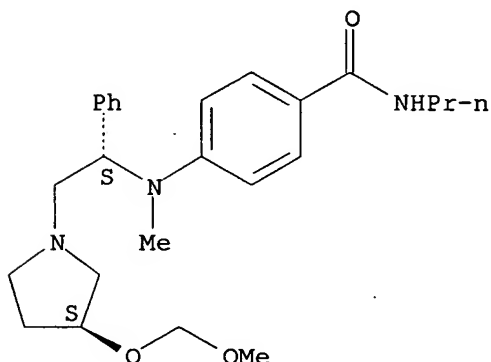
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrrolidinyl- and pyrrolinylethylamines as kappa agonists)

RN 204970-95-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

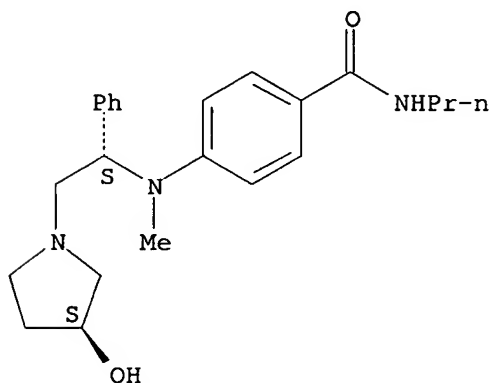
Absolute stereochemistry.



RN 204970-97-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

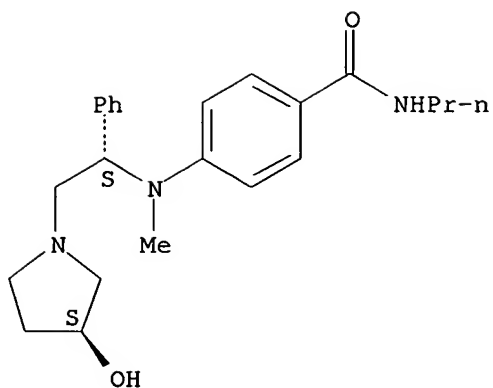


RN 204970-99-0 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



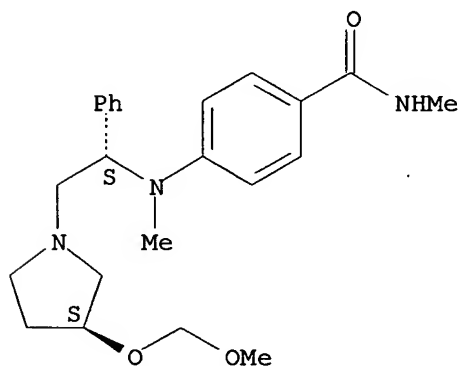


● HCl

RN 204971-01-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl- (9CI) (CA INDEX NAME)

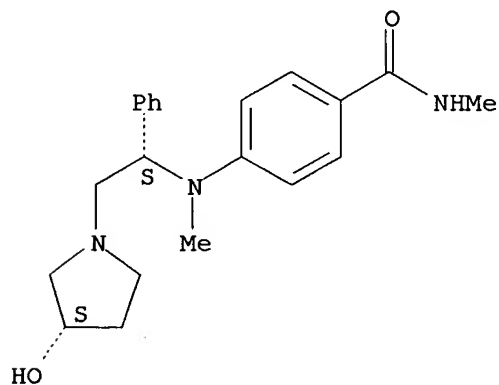
Absolute stereochemistry.



RN 204971-03-9 CAPLUS

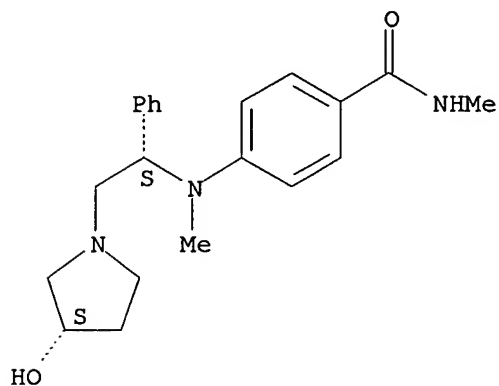
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-05-1 CAPLUS  
CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

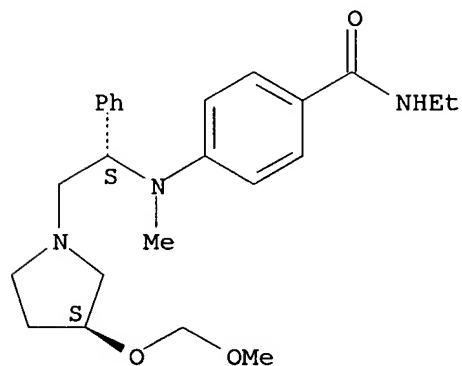
Absolute stereochemistry.



● HCl

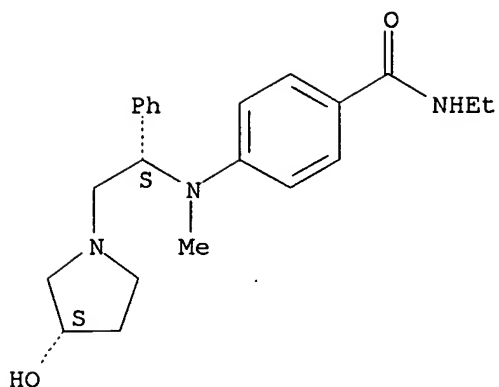
RN 204971-07-3 CAPLUS  
CN Benzamide, N-ethyl-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-09-5 CAPLUS  
CN Benzamide, N-ethyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

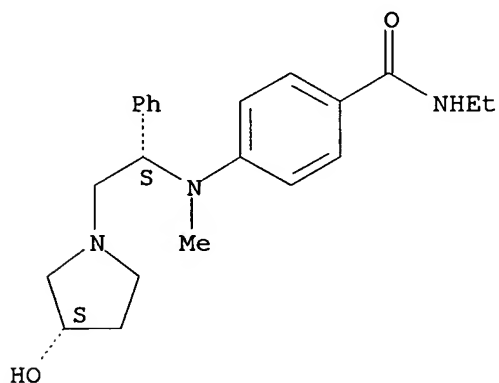
Absolute stereochemistry.



RN 204971-11-9 CAPLUS

CN Benzamide, N-ethyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

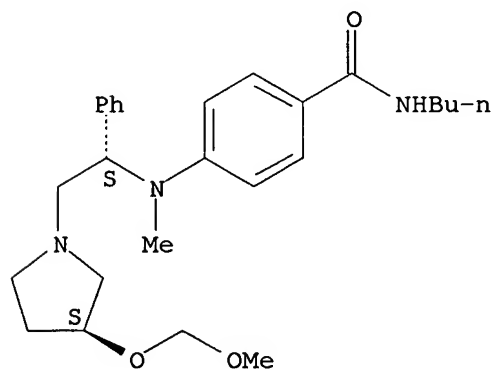


● HCl

RN 204971-13-1 CAPLUS

CN Benzamide, N-butyl-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

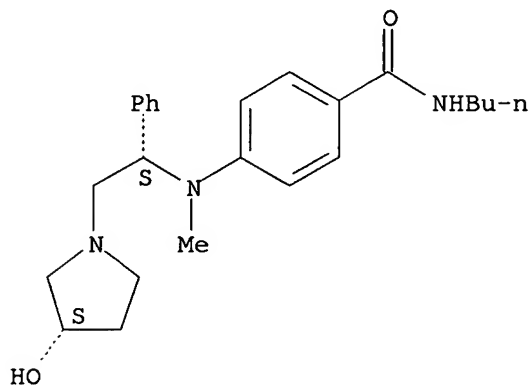
Absolute stereochemistry.



RN 204971-15-3 CAPLUS

CN Benzamide, N-butyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

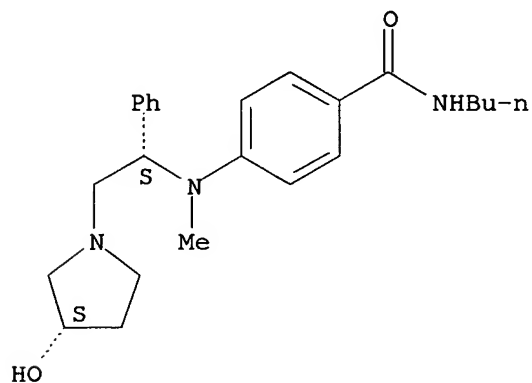
Absolute stereochemistry.



RN 204971-17-5 CAPLUS

CN Benzamide, N-butyl-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

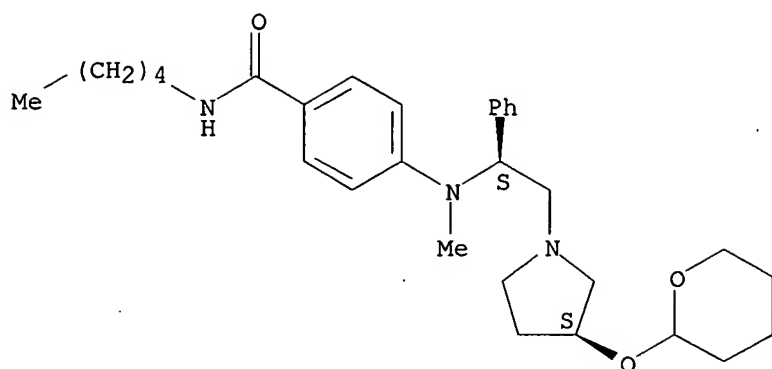


● HCl

RN 204971-19-7 CAPLUS

CN Benzamide, 4-[methyl[(1S)-1-phenyl-2-[(3S)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-1-pyrrolidinyl]ethyl]amino]-N-pentyl- (9CI) (CA INDEX NAME)

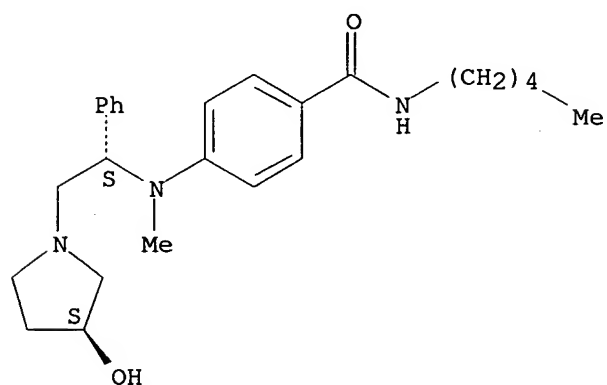
Absolute stereochemistry.



RN 204971-21-1 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-pentyl- (9CI) (CA INDEX NAME)

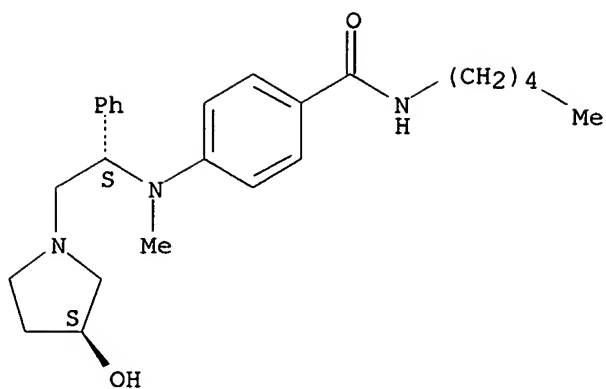
Absolute stereochemistry.



RN 204971-23-3 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-pentyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

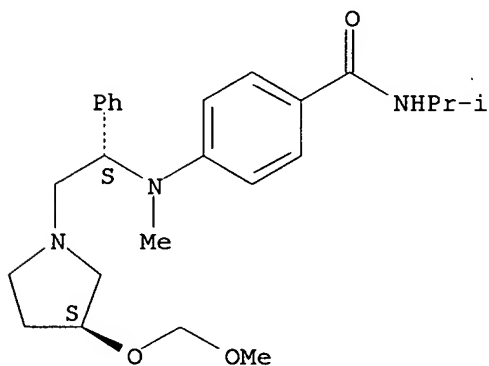


● HCl

RN 204971-25-5 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

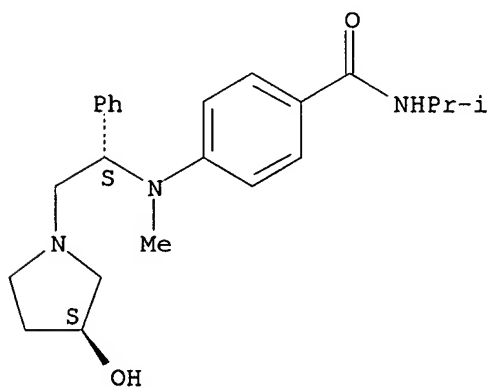
Absolute stereochemistry.



RN 204971-27-7 CAPLUS

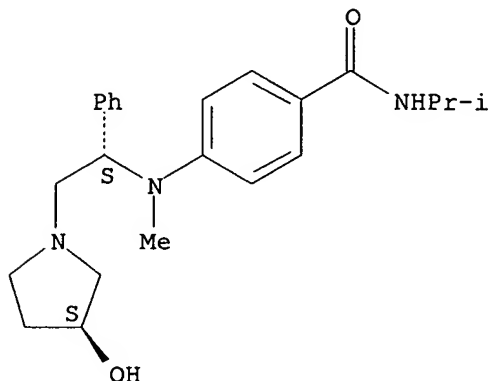
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-29-9 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(1-methylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

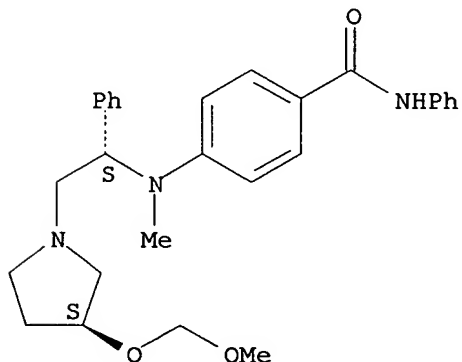
Absolute stereochemistry.



● HCl

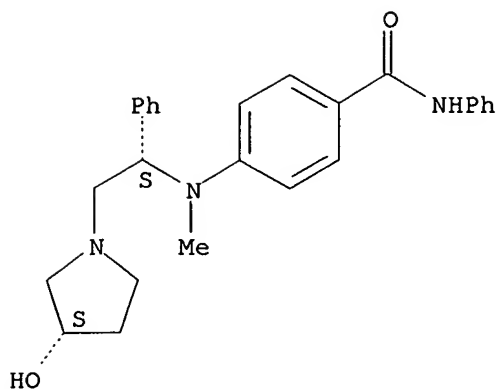
RN 204971-30-2 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-32-4 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-phenyl- (9CI) (CA INDEX NAME)

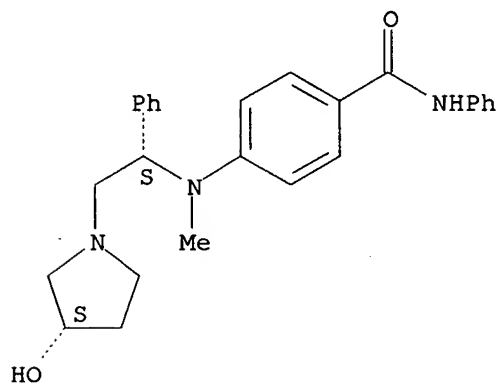
Absolute stereochemistry.



RN 204971-34-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

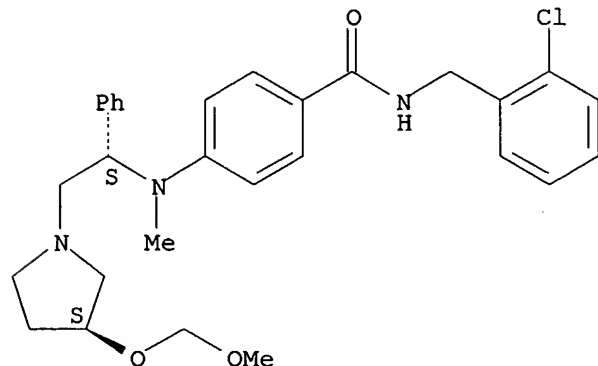


● HCl

RN 204971-36-8 CAPLUS

CN Benzamide, N-[(2-chlorophenyl)methyl]-4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

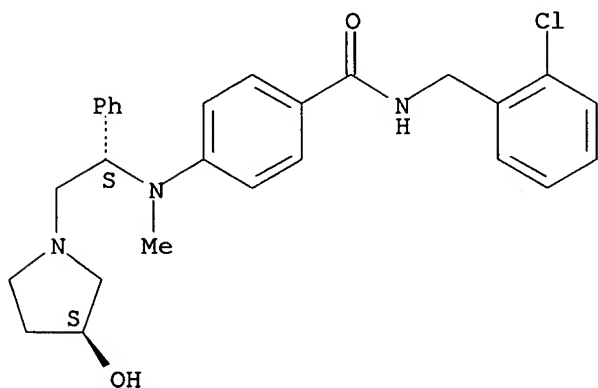




RN 204971-38-0 CAPLUS

CN Benzamide, N-[(2-chlorophenyl)methyl]-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

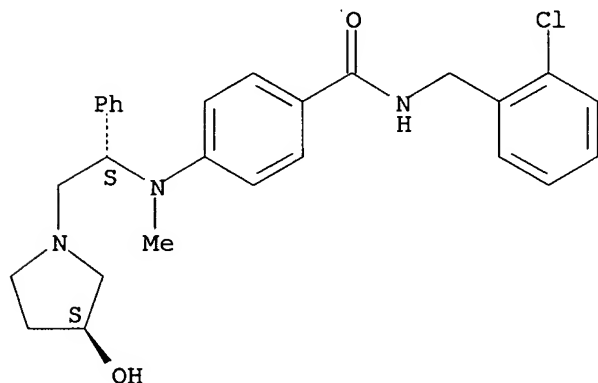
Absolute stereochemistry.



RN 204971-40-4 CAPLUS

CN Benzamide, N-[(2-chlorophenyl)methyl]-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

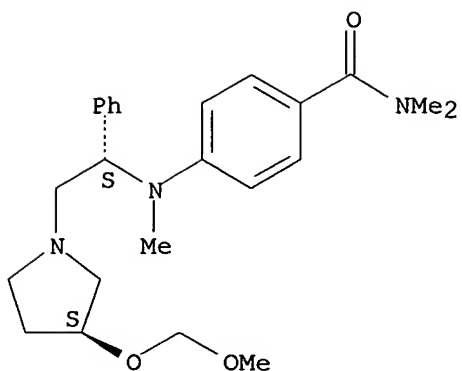


● HCl

RN 204971-42-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N,N-dimethyl]- (9CI) (CA INDEX NAME)

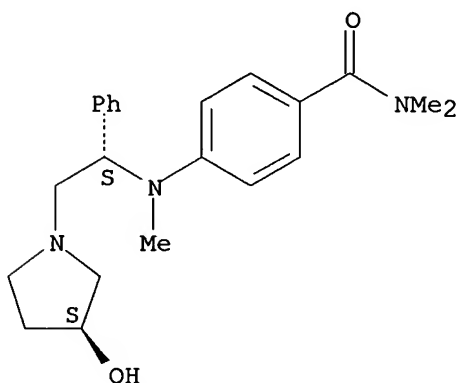
Absolute stereochemistry.



RN 204971-44-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

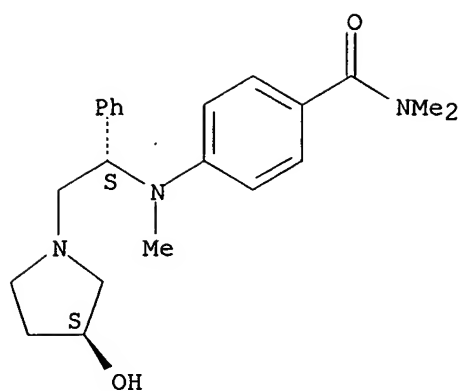
Absolute stereochemistry.



RN 204971-46-0 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N,N-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

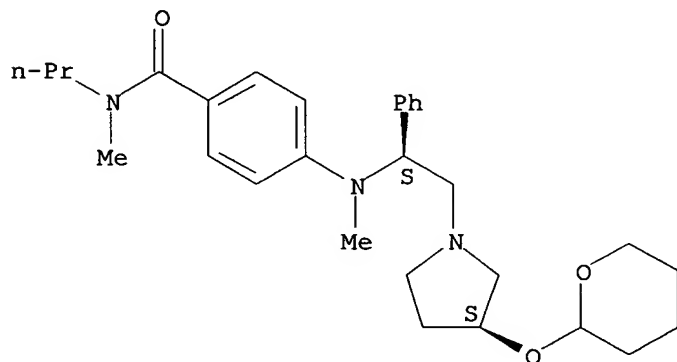


● HCl

RN 204971-48-2 CAPLUS

CN Benzamide, N-methyl-4-[methyl[(1S)-1-phenyl-2-[(3S)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-1-pyrrolidinyl]ethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

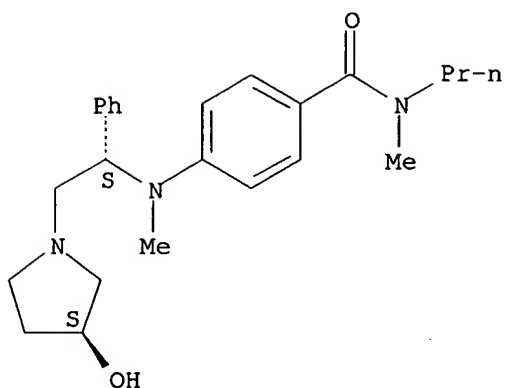
Absolute stereochemistry.



RN 204971-50-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl-N-propyl- (9CI) (CA INDEX NAME)

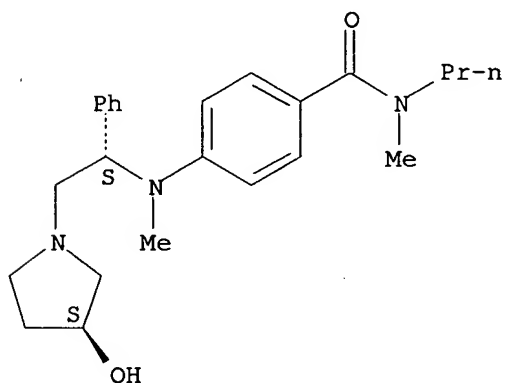
Absolute stereochemistry.



RN 204971-52-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-methyl-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

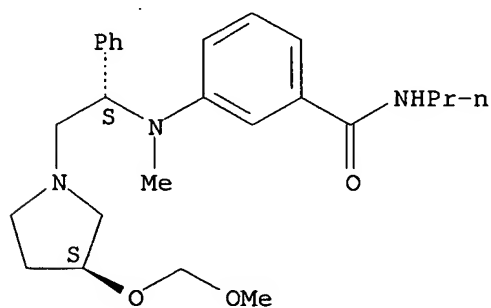


● HCl

RN 204971-54-0 CAPLUS

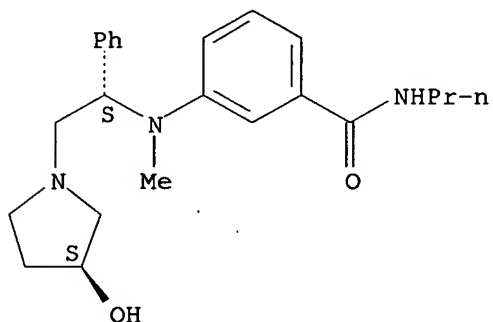
CN Benzamide, 3-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



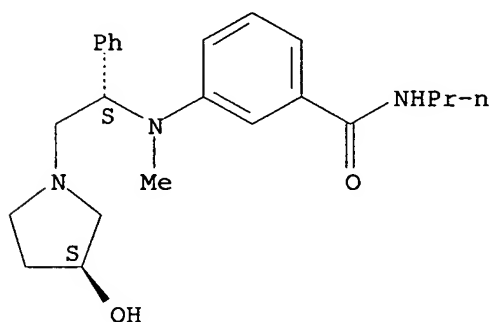
RN 204971-56-2 CAPLUS  
CN Benzamide, 3-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-58-4 CAPLUS  
CN Benzamide, 3-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

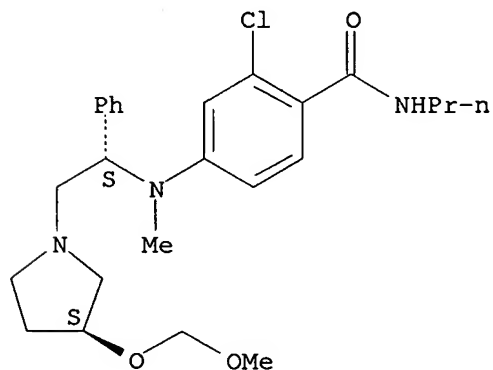
Absolute stereochemistry.



● HCl

RN 204971-60-8 CAPLUS  
CN Benzamide, 2-chloro-4-[[2-[3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

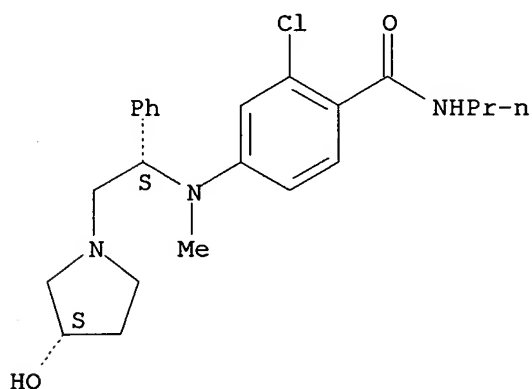
Absolute stereochemistry.



RN 204971-61-9 CAPLUS

CN Benzamide, 2-chloro-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

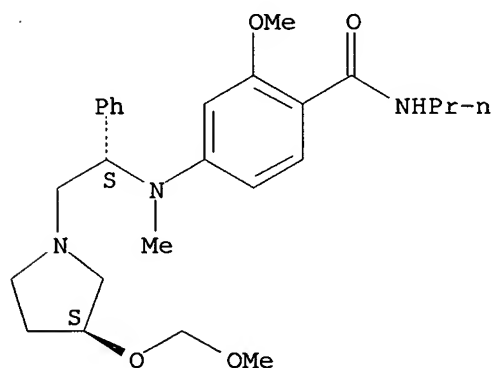
Absolute stereochemistry.



RN 204971-62-0 CAPLUS

CN Benzamide, 2-methoxy-4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

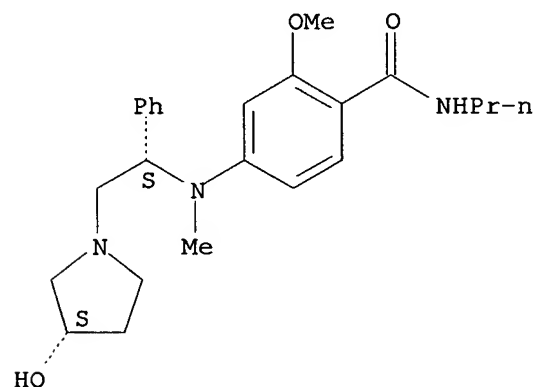
Absolute stereochemistry.



RN 204971-64-2 CAPLUS

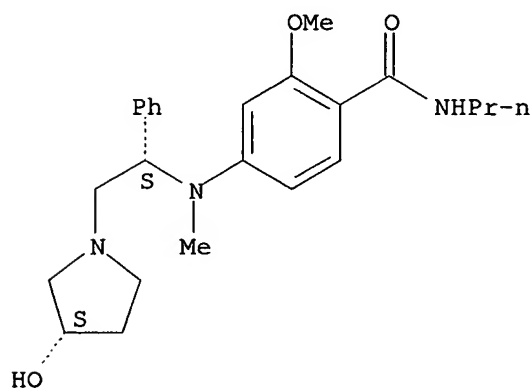
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-2-methoxy-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-66-4 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-2-methoxy-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

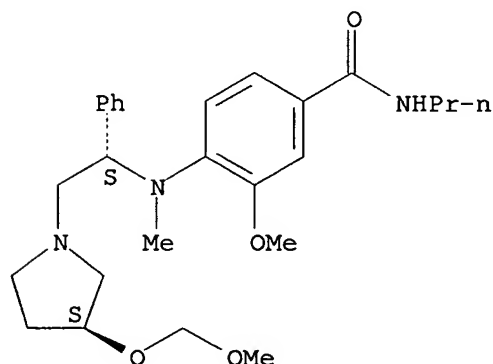
Absolute stereochemistry.



● HCl

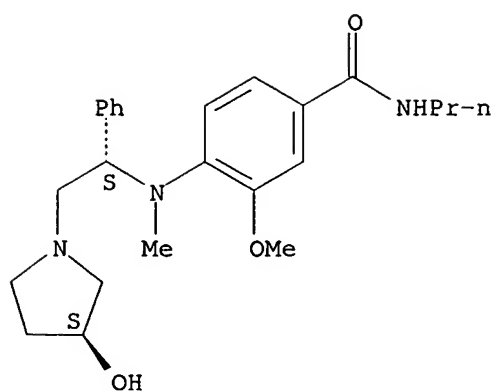
RN 204971-67-5 CAPLUS  
CN Benzamide, 3-methoxy-4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-68-6 CAPLUS  
CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-3-methoxy-N-propyl- (9CI) (CA INDEX NAME)

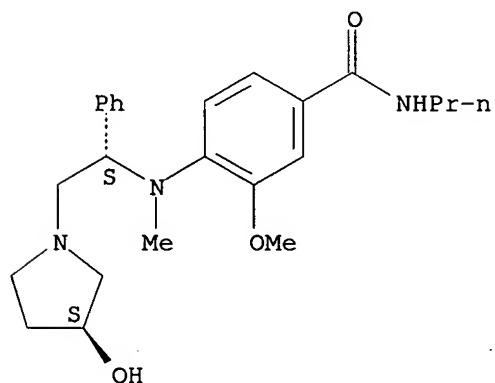
Absolute stereochemistry.



RN 204971-69-7 CAPLUS

CN Benzamide, 4-[[1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-3-methoxy-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



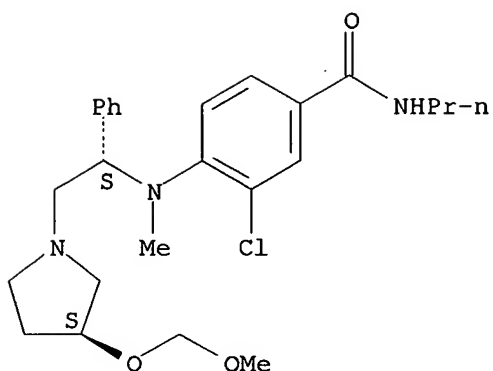
● HCl

RN 204971-70-0 CAPLUS

CN Benzamide, 3-chloro-4-[[1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

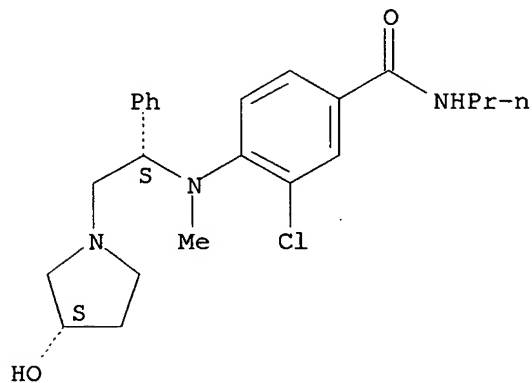




RN 204971-71-1 CAPLUS

CN Benzamide, 3-chloro-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-72-2 CAPLUS

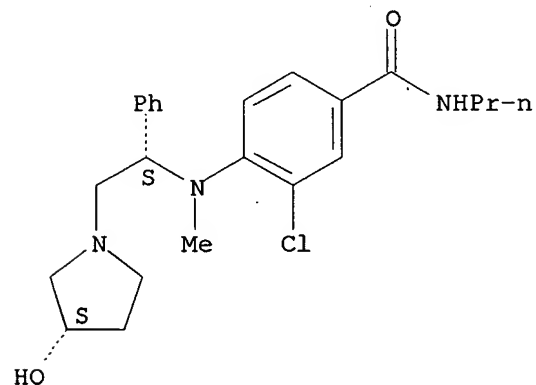
CN Benzamide, 3-chloro-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204971-71-1

CMF C23 H30 Cl N3 O2

Absolute stereochemistry.

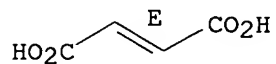


CM 2

CRN 110-17-8

CMF C4 H4 O4

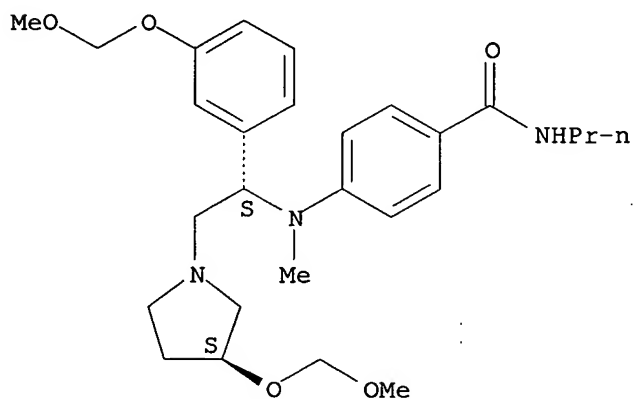
Double bond geometry as shown.



RN 204971-76-6 CAPLUS

CN Benzamide, 4-[[[(1S)-1-[3-(methoxymethoxy)phenyl]-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

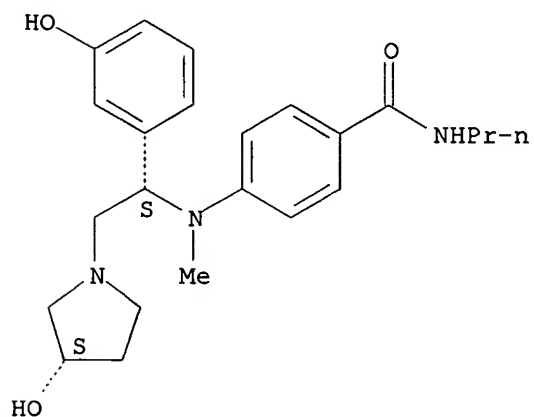
Absolute stereochemistry.



RN 204971-77-7 CAPLUS

CN Benzamide, 4-[[[(1S)-1-(3-hydroxyphenyl)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

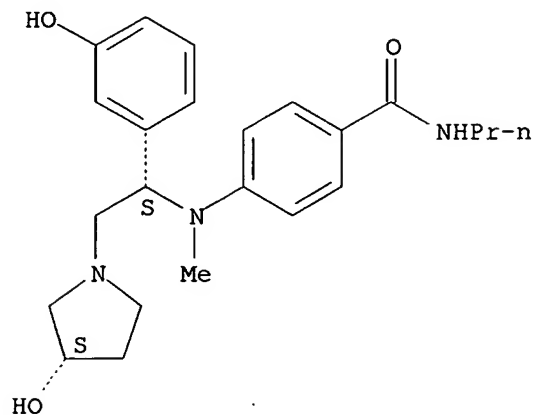
Absolute stereochemistry.



RN 204971-78-8 CAPLUS

CN Benzamide, 4-[[[(1S)-1-(3-hydroxyphenyl)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]ethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

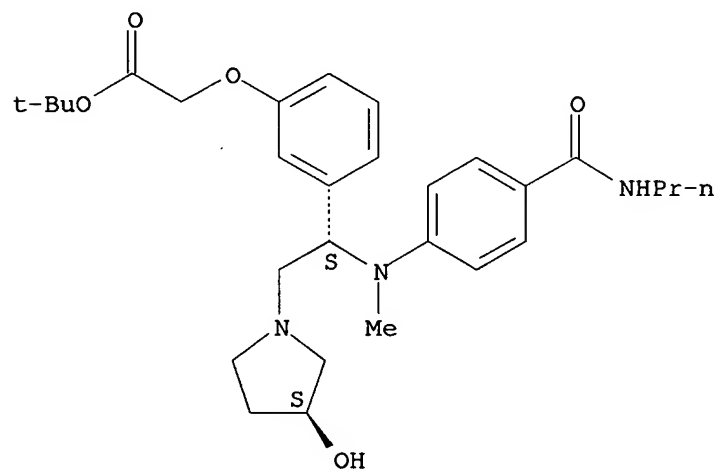


● HCl

RN 204971-79-9 CAPLUS

CN Acetic acid, [3-[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

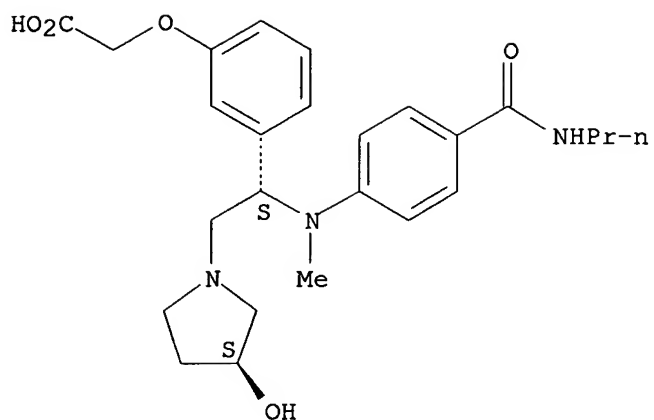
Absolute stereochemistry.



RN 204971-80-2 CAPLUS

CN Acetic acid, [3-[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]- (9CI) (CA INDEX NAME)

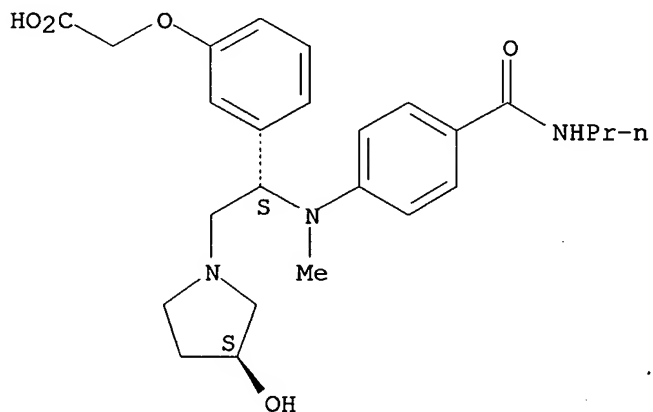
Absolute stereochemistry.



RN 204971-81-3 CAPLUS

CN Acetic acid, [3-[2-(3-hydroxy-1-pyrrolidinyl)-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, monohydrochloride, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

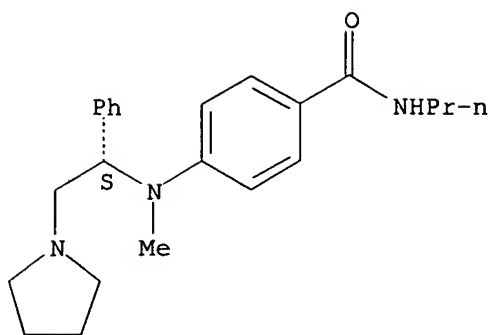


● HCl

RN 204971-82-4 CAPLUS

CN Benzamide, 4-[methyl[(1S)-1-phenyl-2-(1-pyrrolidinyl)ethyl]amino]-N-propyl-, (9CI) (CA INDEX NAME)

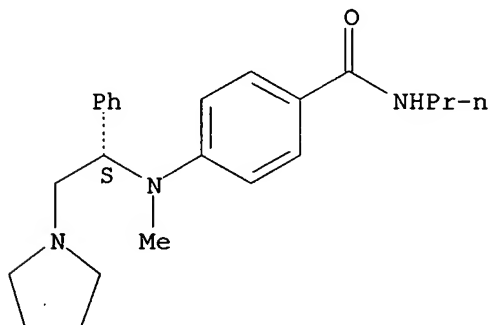
Absolute stereochemistry.



RN 204971-83-5 CAPLUS

CN Benzamide, 4-[methyl[(1S)-1-phenyl-2-(1-pyrrolidinyl)ethyl]amino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

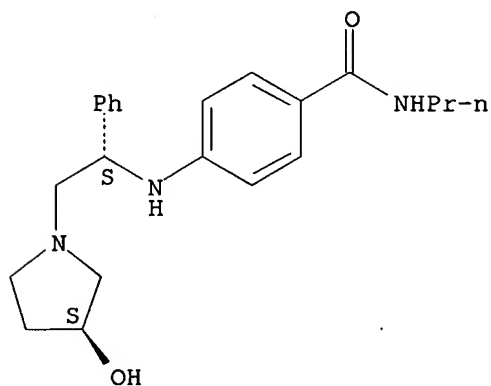


● HCl

RN 204971-89-1 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

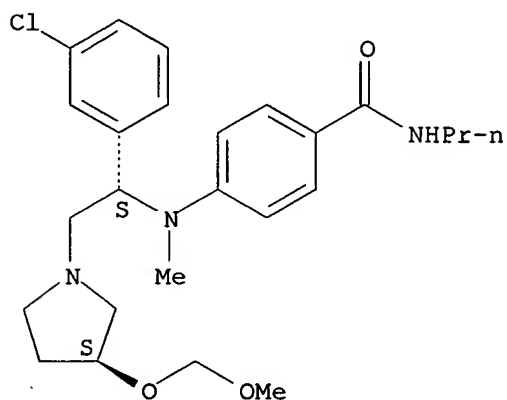


RN 204971-90-4 CAPLUS

CN Benzamide, 4-[[[(1S)-1-(3-chlorophenyl)-2-[(3S)-3-(methoxymethoxy)-1-

pyrrolidinyl]ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

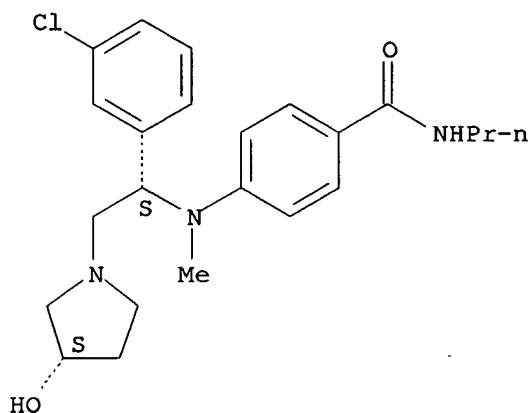
Absolute stereochemistry.



RN 204971-91-5 CAPLUS

CN Benzamide, 4-[[[(1S)-1-(3-chlorophenyl)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-92-6 CAPLUS

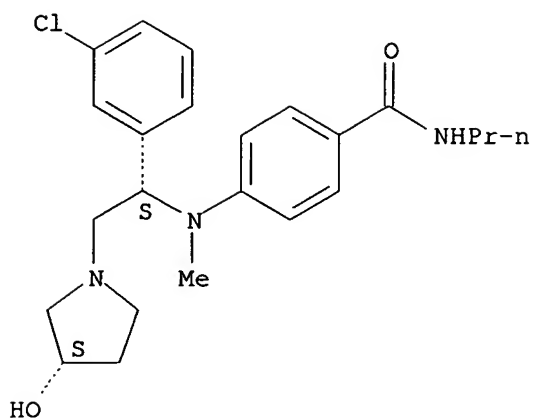
CN Benzamide, 4-[[[(1S)-1-(3-chlorophenyl)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]ethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204971-91-5

CMF C23 H30 Cl N3 O2

Absolute stereochemistry.

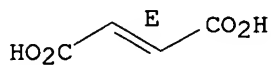


CM 2

CRN 110-17-8

CMF C4 H4 O4

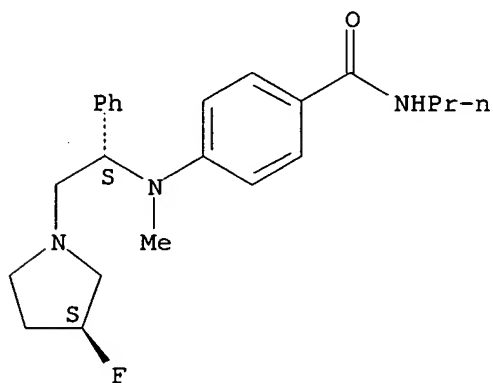
Double bond geometry as shown.



RN 204971-93-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

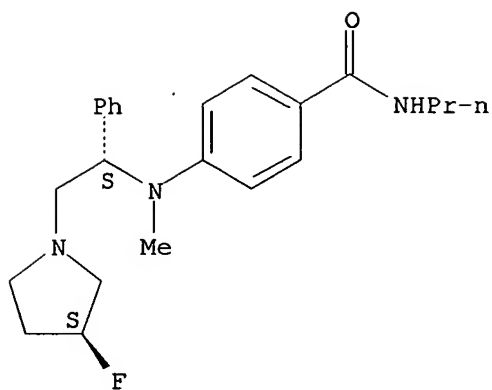
Absolute stereochemistry.



RN 204971-94-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

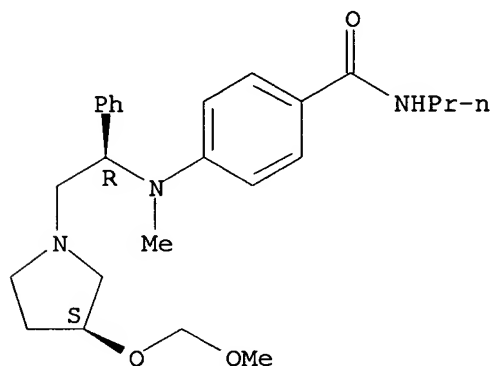
Absolute stereochemistry.



● HCl

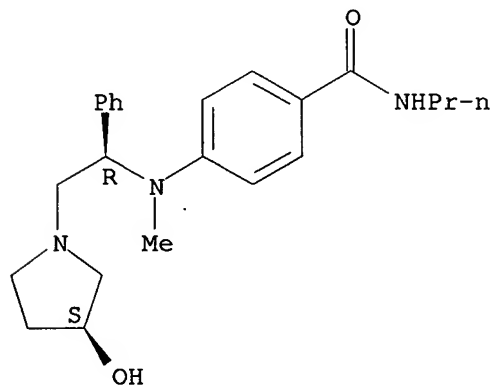
RN 204971-95-9 CAPLUS  
 CN Benzamide, 4-[[[(1R)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204971-96-0 CAPLUS  
 CN Benzamide, 4-[[[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

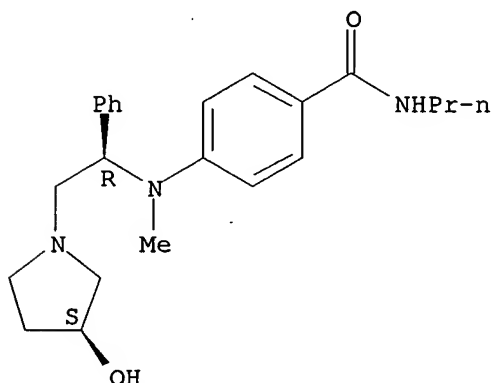
Absolute stereochemistry.





RN 204971-97-1 CAPLUS  
 CN Benzamide, 4-[[[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

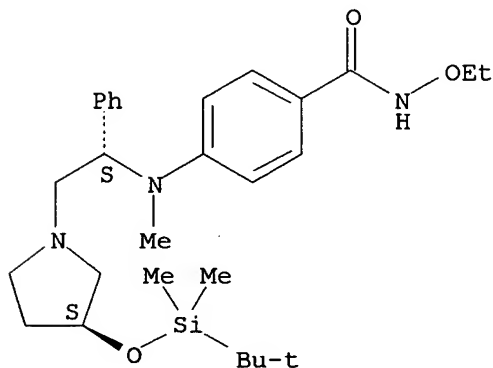
Absolute stereochemistry.



● HCl

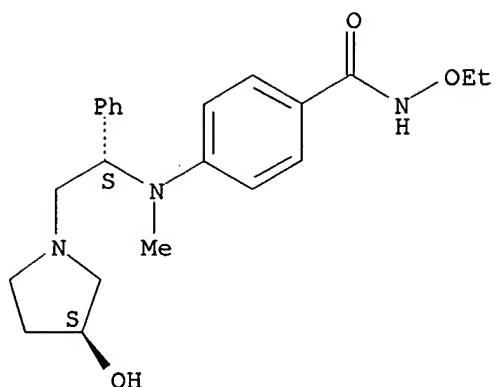
RN 204972-01-0 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-[[[1,1-dimethylethyl]dimethylsilyl]oxy]-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-ethoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-02-1 CAPLUS  
 CN Benzamide, N-ethoxy-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

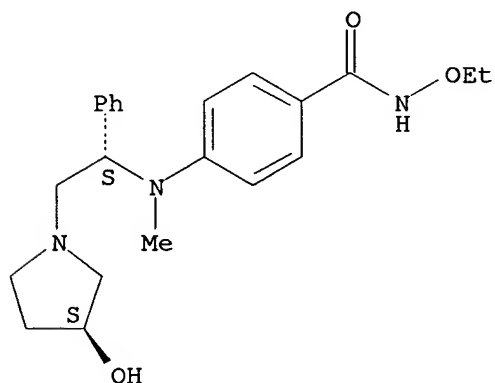
Absolute stereochemistry.



RN 204972-03-2 CAPLUS

CN Benzamide, N-ethoxy-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

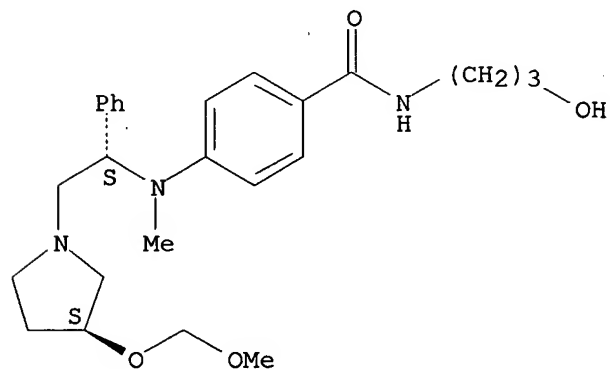


● HCl

RN 204972-07-6 CAPLUS

CN Benzamide, N-(3-hydroxypropyl)-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

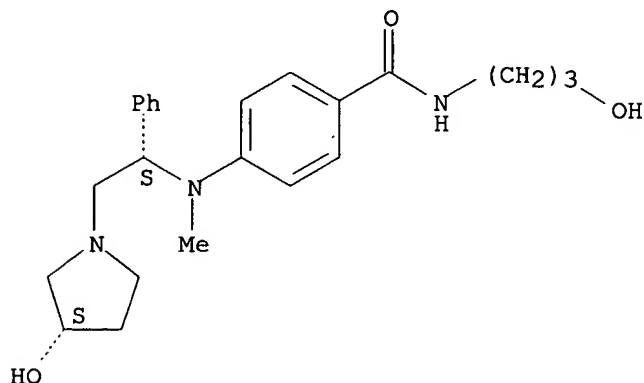
Absolute stereochemistry.



RN 204972-08-7 CAPLUS

CN Benzamide, N-(3-hydroxypropyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

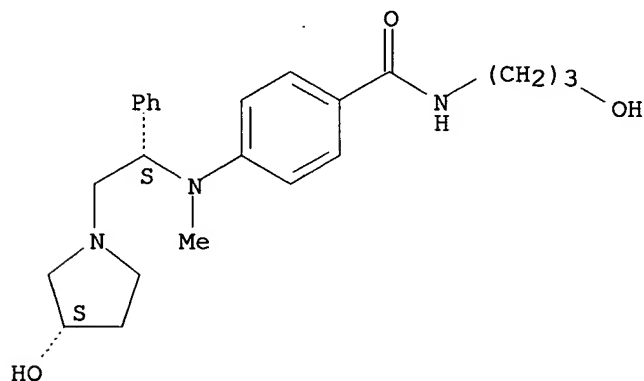
Absolute stereochemistry.



RN 204972-09-8 CAPLUS

CN Benzamide, N-(3-hydroxypropyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

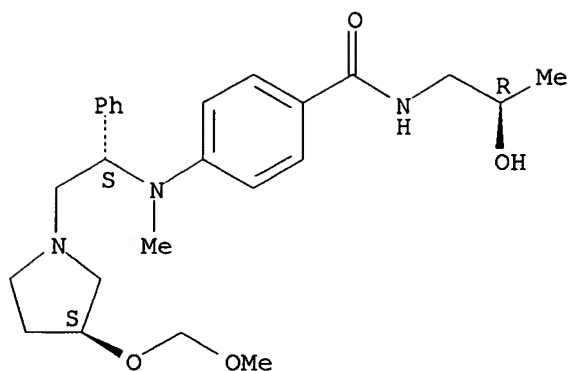


● HCl

RN 204972-10-1 CAPLUS

CN Benzamide, N-[(2R)-2-hydroxypropyl]-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

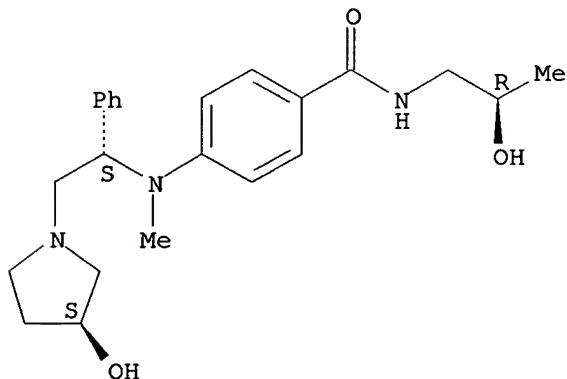
Absolute stereochemistry.



RN 204972-11-2 CAPLUS

CN Benzamide, N-[(2R)-2-hydroxypropyl]-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

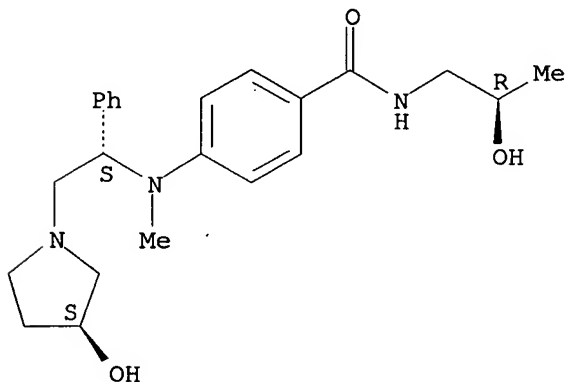
Absolute stereochemistry.



RN 204972-12-3 CAPLUS

CN Benzamide, N-[(2R)-2-hydroxypropyl]-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

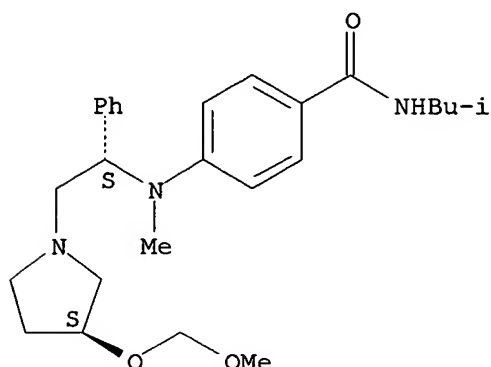


● HCl

RN 204972-13-4 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

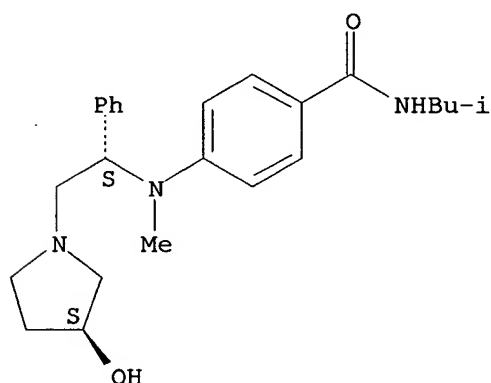
Absolute stereochemistry.



RN 204972-14-5 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

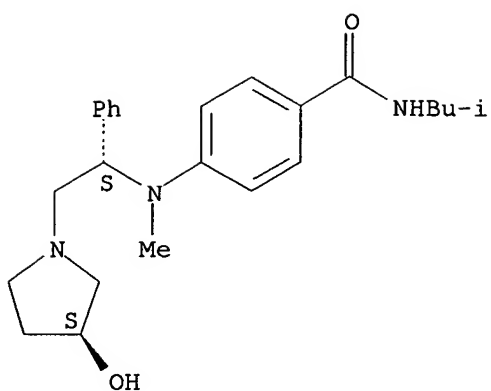
Absolute stereochemistry.



RN 204972-15-6 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2-methylpropyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

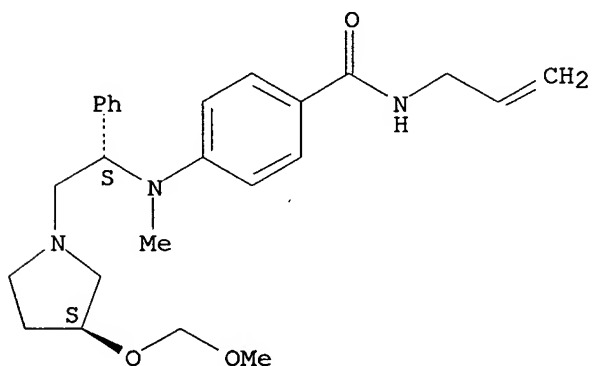


● HCl

RN 204972-16-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propenyl- (9CI) (CA INDEX NAME)

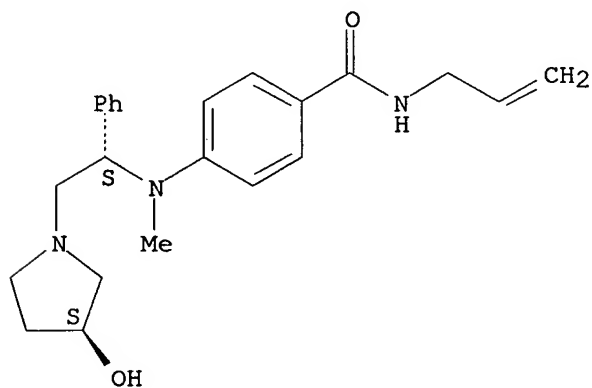
Absolute stereochemistry.



RN 204972-17-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propenyl- (9CI) (CA INDEX NAME)

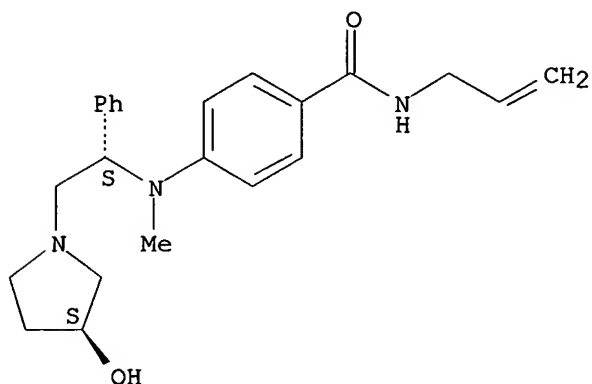
Absolute stereochemistry.



RN 204972-18-9 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propenyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

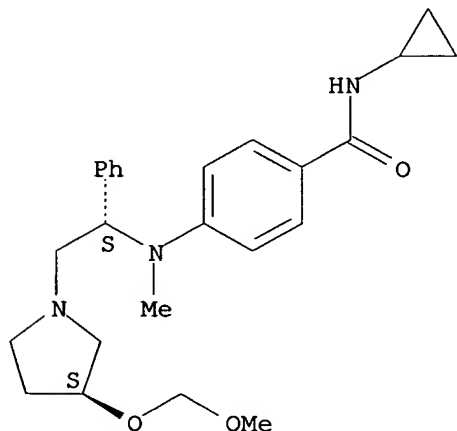


● HCl

RN 204972-19-0 CAPLUS

CN Benzamide, N-cyclopropyl-4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

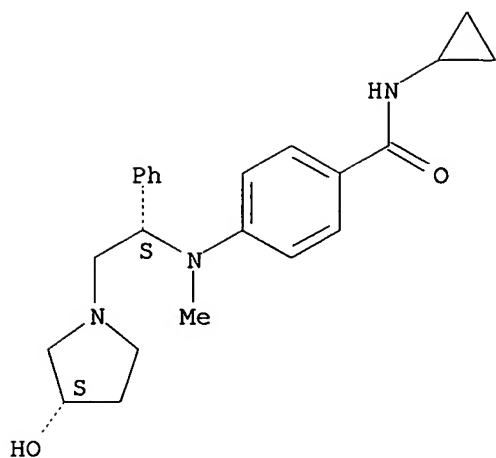
Absolute stereochemistry.



RN 204972-20-3 CAPLUS

CN Benzamide, N-cyclopropyl-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

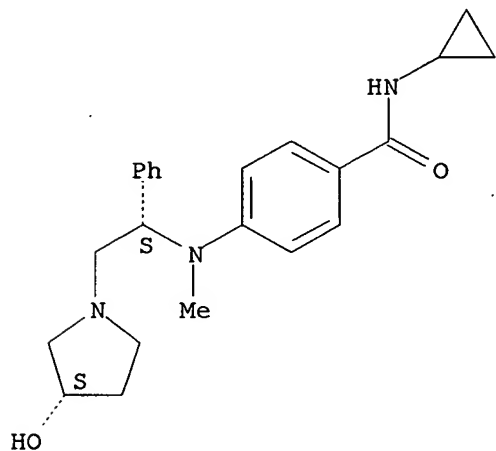
Absolute stereochemistry.



RN 204972-21-4 CAPLUS

CN Benzamide, N-cyclopropyl-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



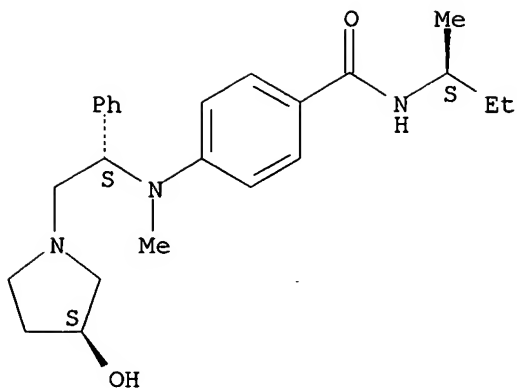
● HCl

RN 204972-22-5 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1S)-1-methylpropyl]- (9CI) (CA INDEX NAME)

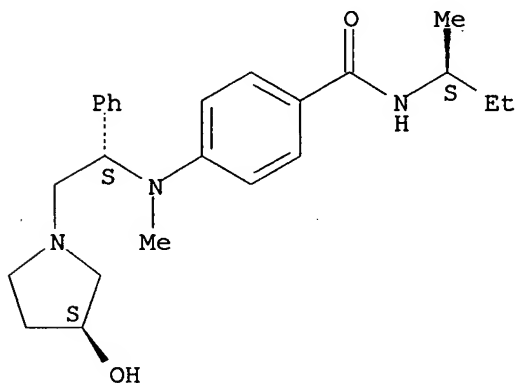
Absolute stereochemistry.





RN 204972-23-6 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1S)-1-methylpropyl]-, monohydrochloride (9CI)  
 (CA INDEX NAME)

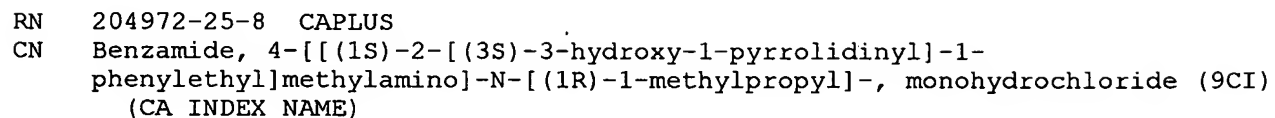
Absolute stereochemistry.



● HCl

RN 204972-24-7 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1R)-1-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

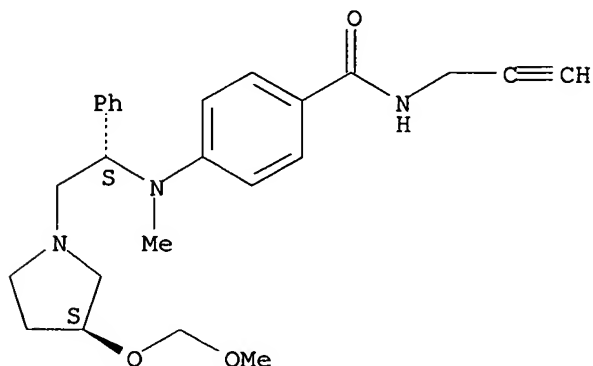


RN	204972-26-9	CAPLUS
CN	Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(1R)-1-methylpropyl]- (9CI) (CA INDEX NAME)	

RN 204972-27-0 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propynyl- (9CI) (CA INDEX NAME)

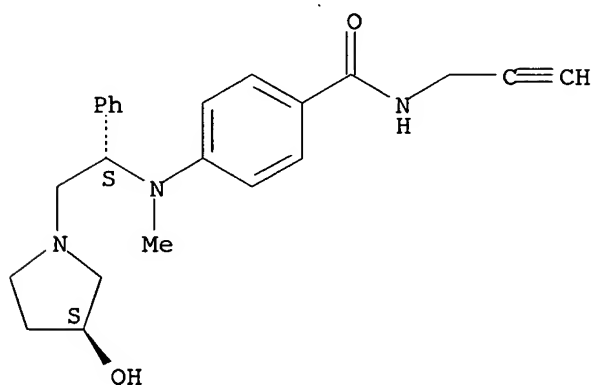
Absolute stereochemistry.



RN 204972-28-1 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propynyl- (9CI) (CA INDEX NAME)

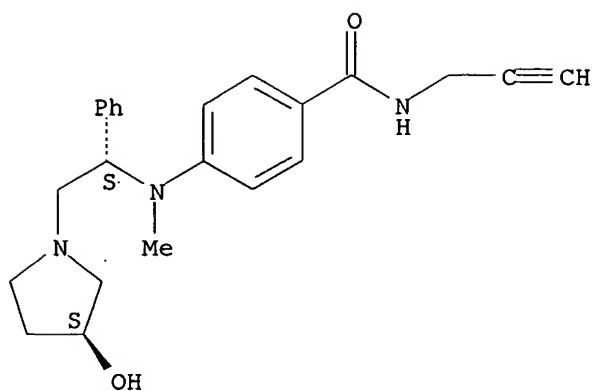
Absolute stereochemistry.



RN 204972-29-2 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-2-propynyl-, monohydrochloride (9CI) (CA INDEX NAME)

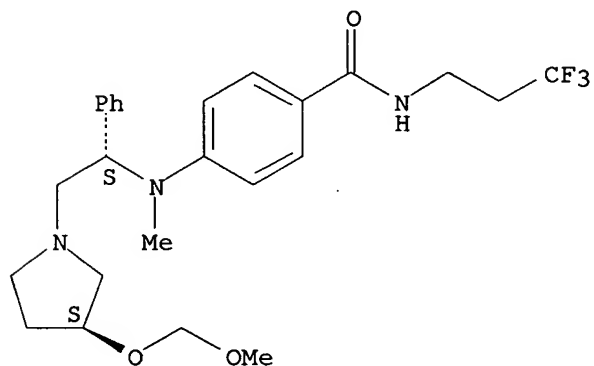
Absolute stereochemistry.



● HCl

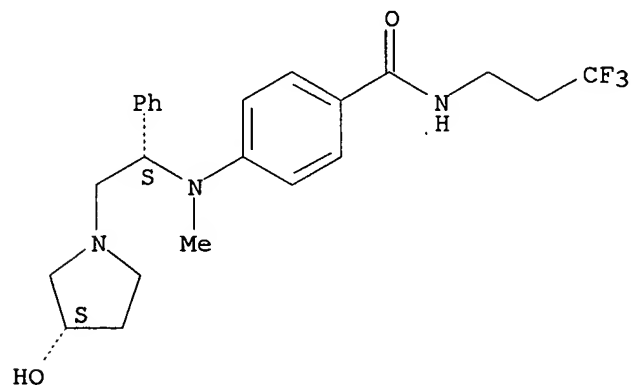
RN 204972-30-5 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



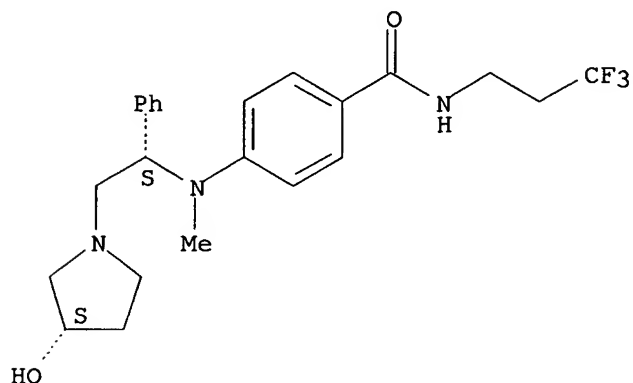
RN 204972-31-6 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-32-7 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(3,3,3-trifluoropropyl)-, monohydrochloride (9CI) (CA INDEX NAME)

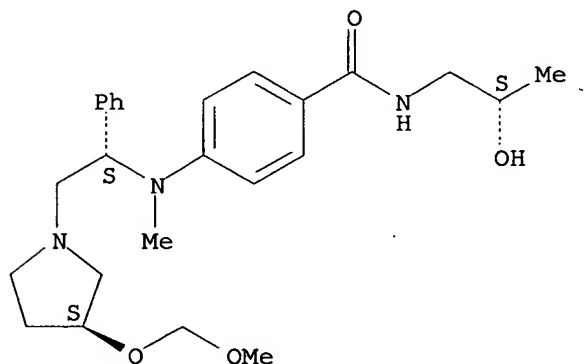
Absolute stereochemistry.



● HCl

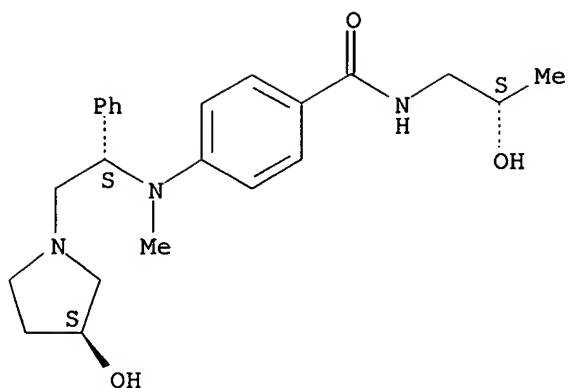
RN 204972-33-8 CAPLUS  
 CN Benzamide, N-[(2S)-2-hydroxypropyl]-4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-34-9 CAPLUS  
 CN Benzamide, N-[(2S)-2-hydroxypropyl]-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-35-0 CAPLUS

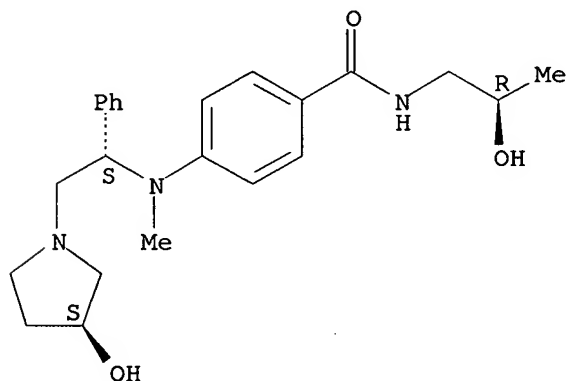
CN Benzamide, N-[(2S)-2-hydroxypropyl]-4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204972-11-2

CMF C23 H31 N3 O3

Absolute stereochemistry.

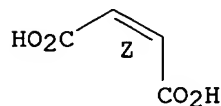


CM 2

CRN 110-16-7

CMF C4 H4 O4

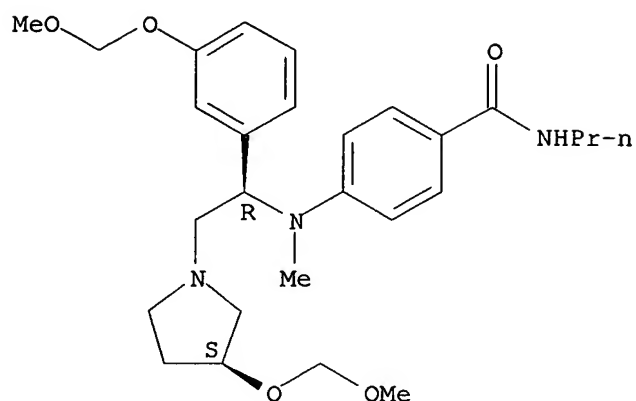
Double bond geometry as shown.



RN 204972-36-1 CAPLUS

CN Benzamide, 4-[[[(1R)-1-[3-(methoxymethoxy)phenyl]-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

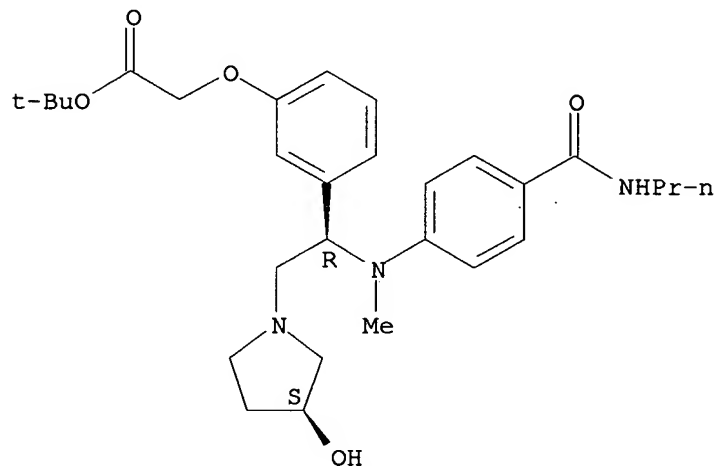
Absolute stereochemistry.



RN 204972-37-2 CAPLUS

CN Acetic acid, [3-[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

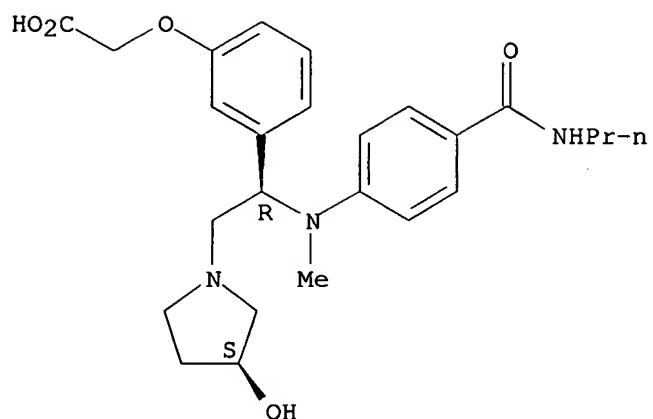
Absolute stereochemistry.



RN 204972-38-3 CAPLUS

CN Acetic acid, [3-[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]- (9CI) (CA INDEX NAME)

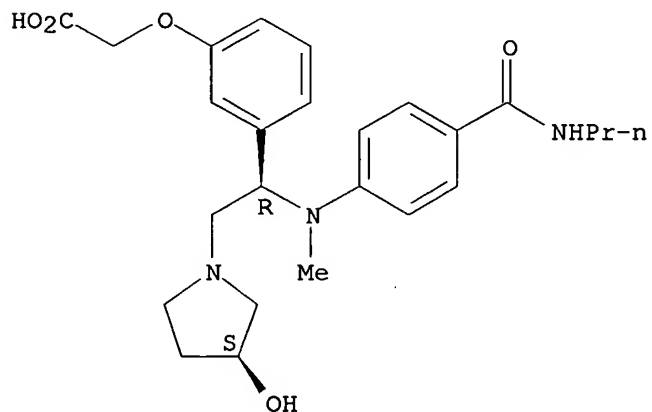
Absolute stereochemistry.



RN 204972-39-4 CAPLUS

CN Acetic acid, [3-[(1R)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



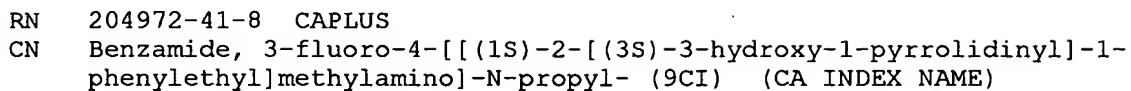
● HCl

RN 204972-40-7 CAPLUS

CN Benzamide, 3-fluoro-4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC(C)NC(=O)c1ccc(N(C)CSCCN2CCCC2S)cc1F

CRN 204972-41-8  
CMF C23 H30 F N3 O2

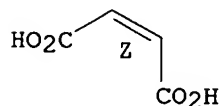
CC(C)NC(=O)c1ccc(N(C)CSCC2CCCN2C3CCCCC3)cc1F

CM 2

CRN 110-16-7

CMF C4 H4 O4

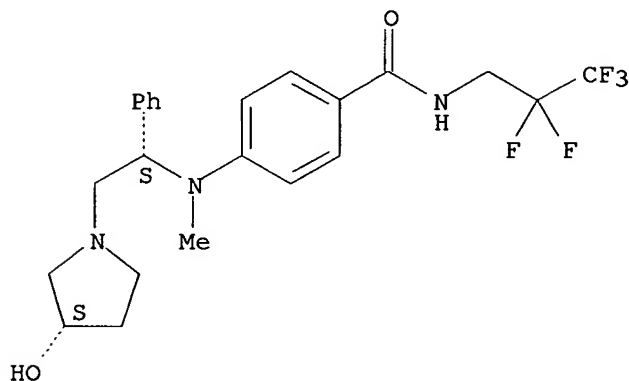
Double bond geometry as shown.



RN 204972-43-0 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

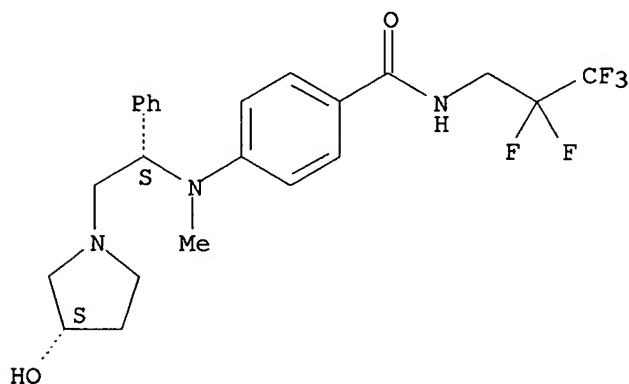
Absolute stereochemistry.



RN 204972-44-1 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2,2,3,3,3-pentafluoropropyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

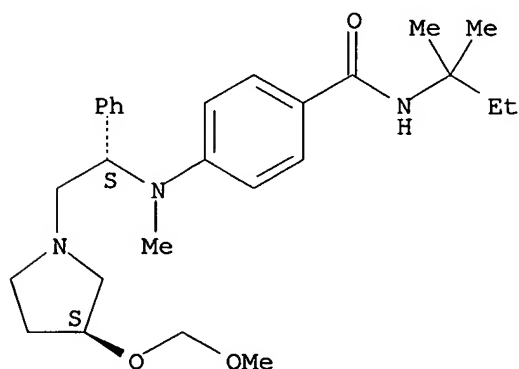


● HCl

RN 204972-45-2 CAPLUS

CN Benzamide, N-(1,1-dimethylpropyl)-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

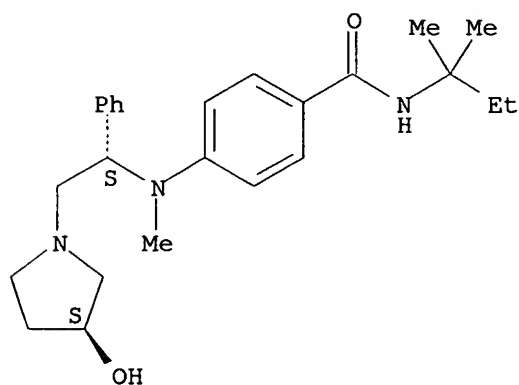
Absolute stereochemistry.



RN 204972-46-3 CAPLUS

CN Benzamide, N-(1,1-dimethylpropyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

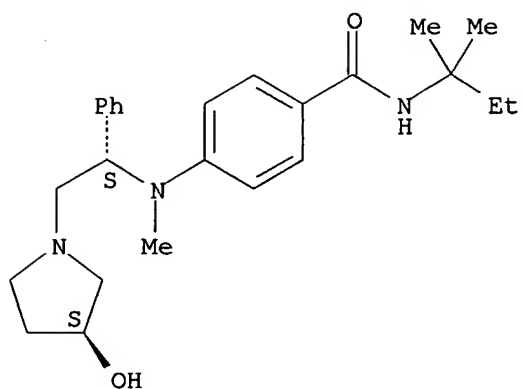
Absolute stereochemistry.



RN 204972-47-4 CAPLUS

CN Benzamide, N-(1,1-dimethylpropyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

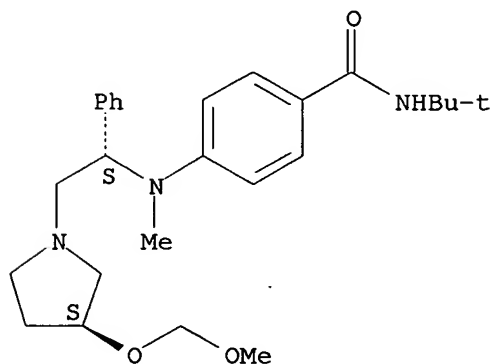


● HCl

RN 204972-48-5 CAPLUS

CN Benzamide, N-(1,1-dimethylethyl)-4-[[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

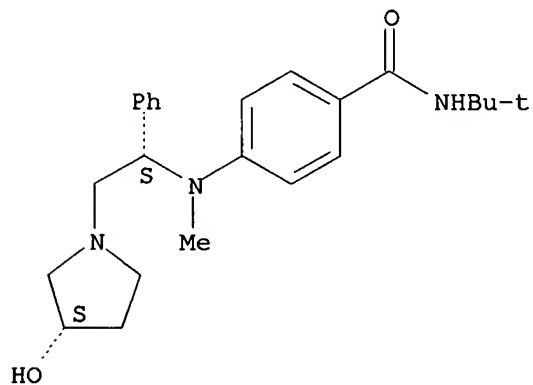
Absolute stereochemistry.



RN 204972-49-6 CAPLUS

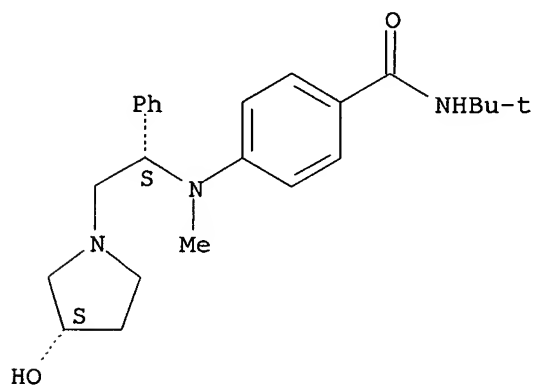
CN Benzamide, N-(1,1-dimethylethyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-50-9 CAPLUS  
 CN Benzamide, N-(1,1-dimethylethyl)-4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]methylamino]-, monohydrochloride (9CI) (CA INDEX NAME)

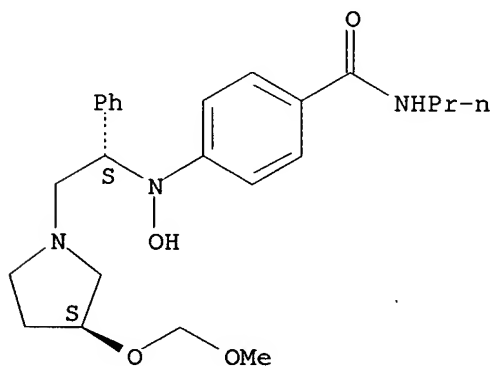
Absolute stereochemistry.



● HCl

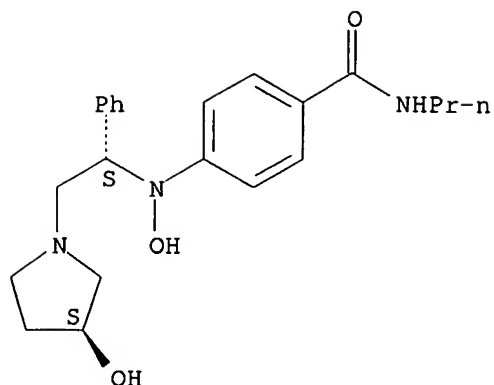
RN 204972-53-2 CAPLUS  
 CN Benzamide, 4-[hydroxy[ (1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204972-54-3 CAPLUS  
 CN Benzamide, 4-[hydroxy[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

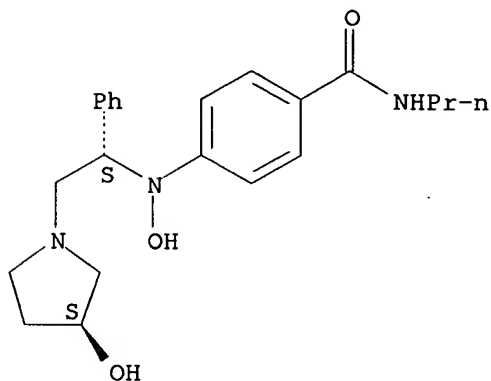


RN 204972-55-4 CAPLUS  
 CN Benzamide, 4-[hydroxy[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204972-54-3  
 CMF C22 H29 N3 O3

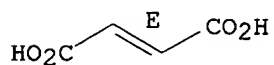
Absolute stereochemistry.



CM 2

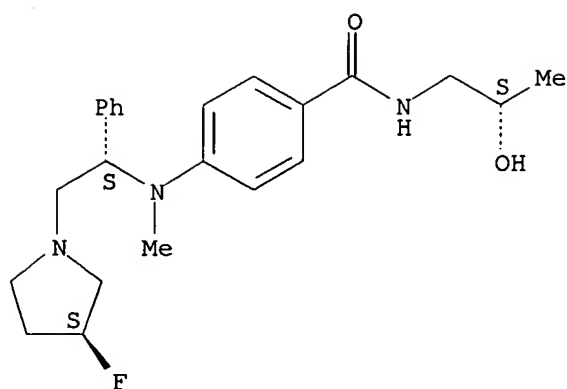
CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



RN 204972-56-5 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2S)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

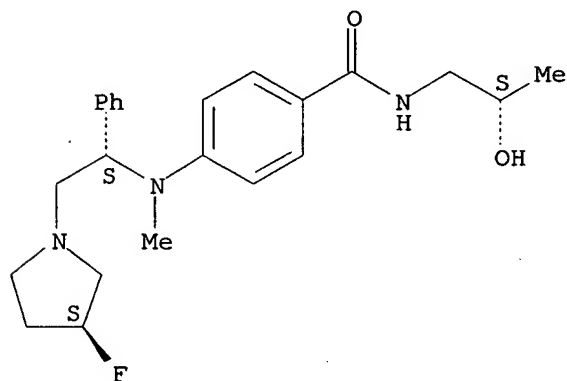


RN 204972-57-6 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2S)-2-hydroxypropyl]-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 204972-56-5  
 CMF C23 H30 F N3 O2

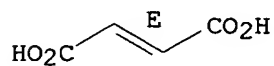
Absolute stereochemistry.



CM 2

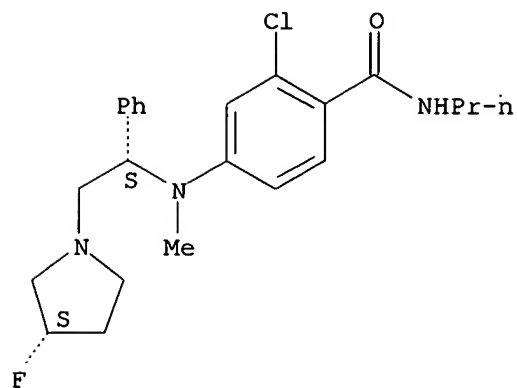
CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



RN 204972-58-7 CAPLUS  
 CN Benzamide, 2-chloro-4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

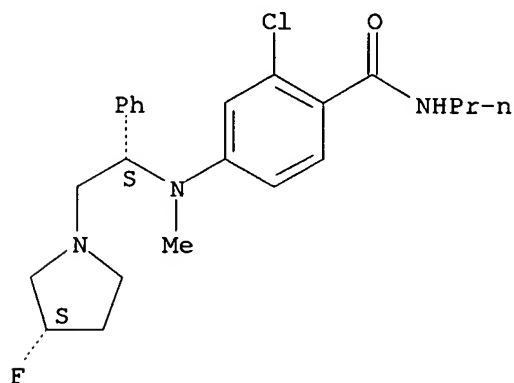


RN 204972-59-8 CAPLUS  
 CN Benzamide, 2-chloro-4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 204972-58-7  
 CMF C23 H29 Cl F N3 O

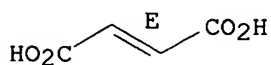
Absolute stereochemistry.



CM 2

CRN 110-17-8  
 CMF C4 H4 O4

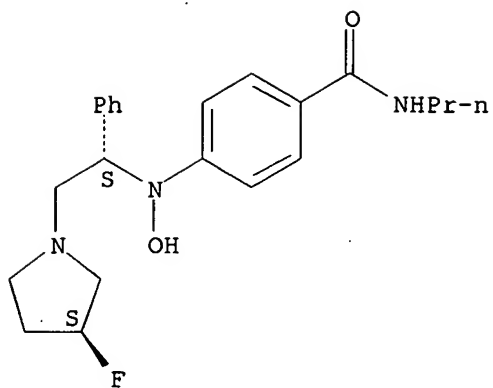
Double bond geometry as shown.



RN 204972-60-1 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]hydroxyamino]-N-propyl- (9CI) (CA INDEX NAME)

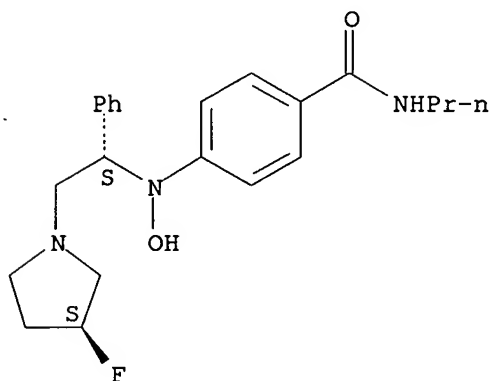
Absolute stereochemistry.





RN 204972-61-2 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]hydroxyamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

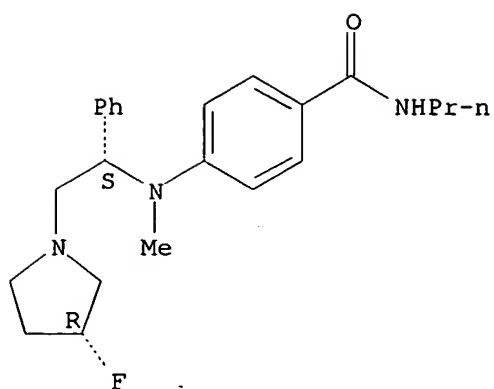
Absolute stereochemistry.



● HCl

RN 204972-66-7 CAPLUS  
 CN Benzamide, 4-[[ (1S)-2-[(3R)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methyamino]-N-propyl- (9CI) (CA INDEX NAME)

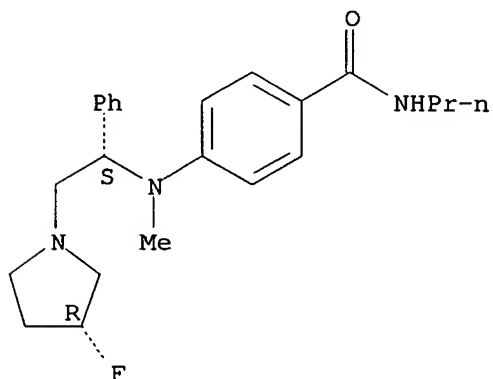
Absolute stereochemistry.



RN 204972-67-8 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3R)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

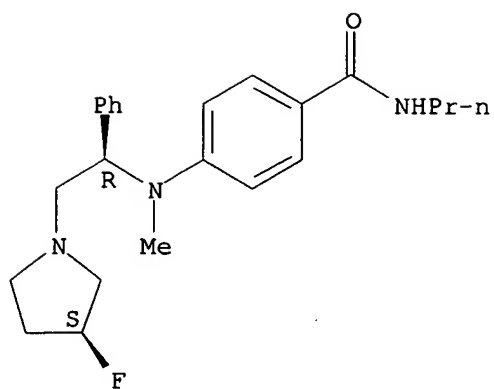


● HCl

RN 204972-68-9 CAPLUS

CN Benzamide, 4-[[[(1R)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

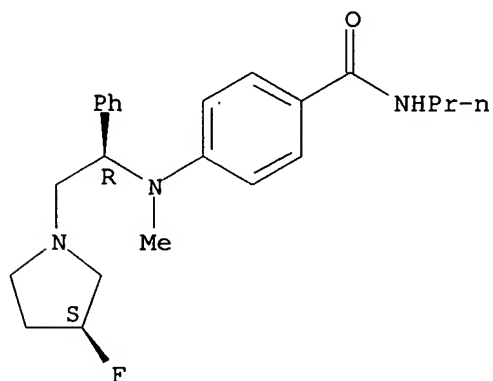
Absolute stereochemistry.



RN 204972-69-0 CAPLUS

CN Benzamide, 4-[[[(1R)-2-[(3S)-3-fluoro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

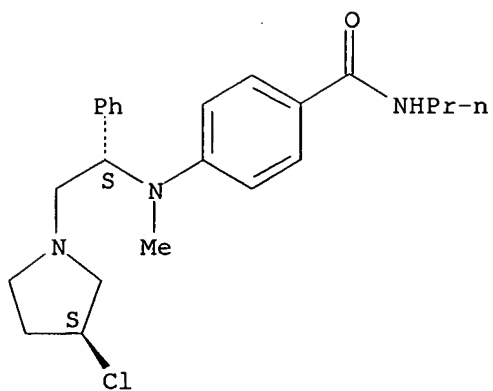


● HCl

RN 204972-70-3 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

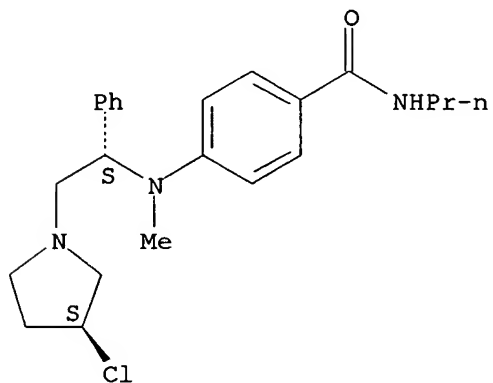
Absolute stereochemistry.



RN 204972-71-4 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

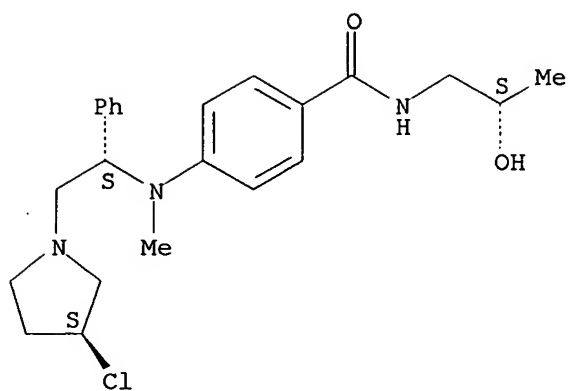


● HCl

RN 204972-72-5 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2S)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

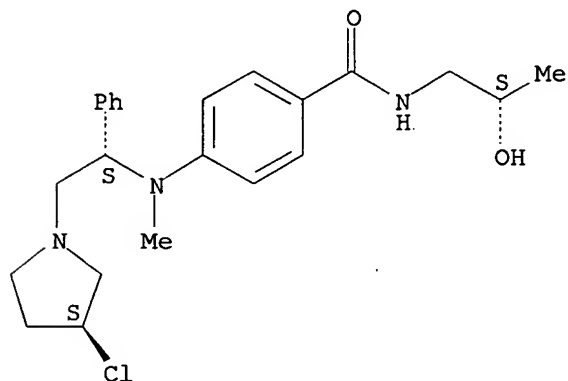
Absolute stereochemistry.



RN 204972-73-6 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2S)-2-hydroxypropyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

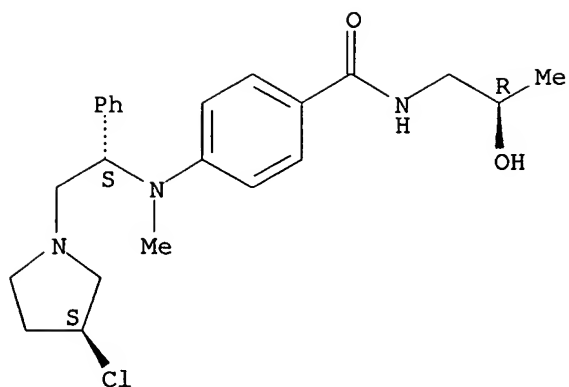


● HCl

RN 204972-74-7 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2R)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

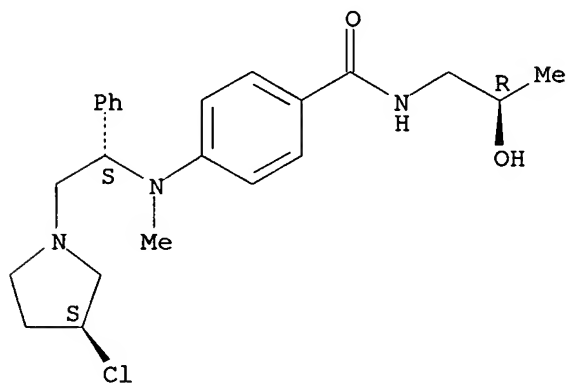
Absolute stereochemistry.



RN 204972-75-8 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-chloro-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-[(2R)-2-hydroxypropyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

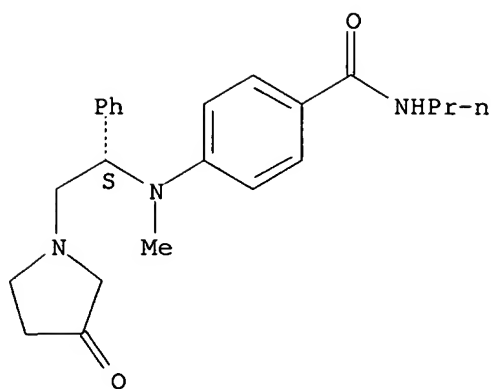


● HCl

RN 204972-76-9 CAPLUS

CN Benzamide, 4-[methyl[(1S)-2-(3-oxo-1-pyrrolidinyl)-1-phenylethyl]amino]-N-propyl- (9CI) (CA INDEX NAME)

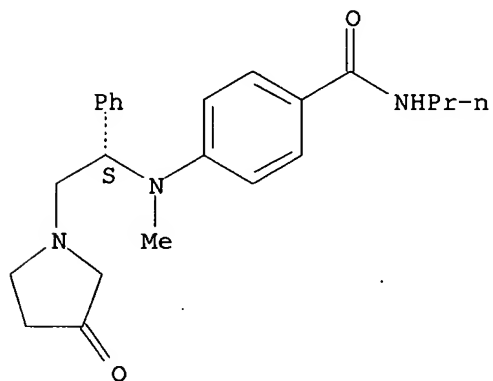
Absolute stereochemistry.



RN 204972-77-0 CAPLUS

CN Benzamide, 4-[methyl[(1S)-2-(3-oxo-1-pyrrolidinyl)-1-phenylethyl]amino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

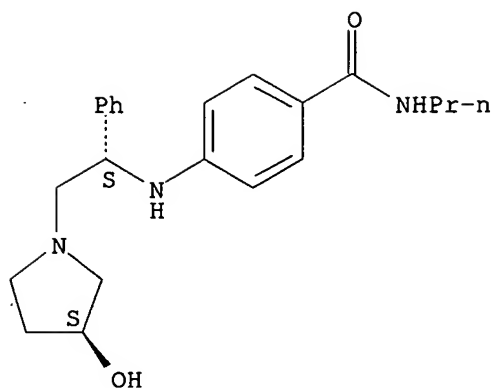


● HCl

RN 204973-49-9 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-phenylethyl]amino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

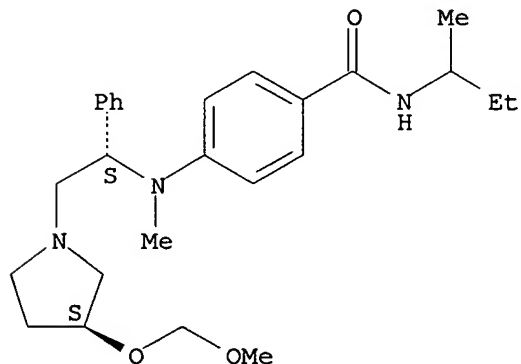


● HCl

RN 204973-50-2 CAPLUS

CN Benzamide, 4-[[2-[3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(1-methylpropyl)-, [3S-[1(1R\*),3R\*]]-[partial]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

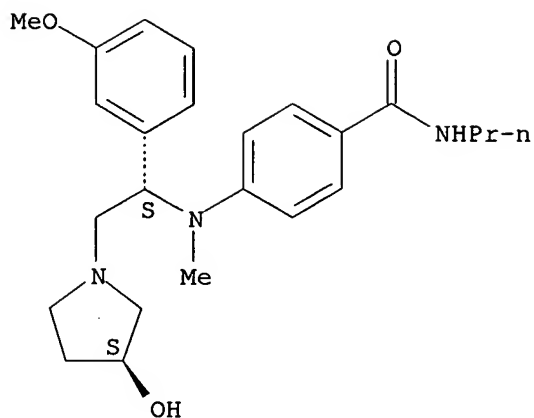


RN 204973-55-7 CAPLUS

CN Benzamide, 4-[[[(1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-(3-methoxyphenyl)ethyl]methylamino]-N-propyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

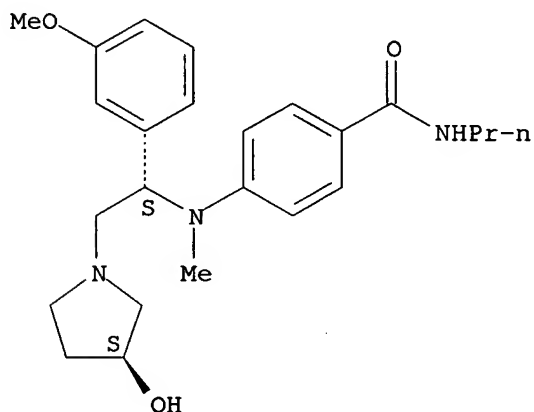




RN 204973-56-8 CAPLUS

CN Benzamide, 4-[[ (1S)-2-[(3S)-3-hydroxy-1-pyrrolidinyl]-1-(3-methoxyphenyl)ethyl]methylamino]-N-propyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

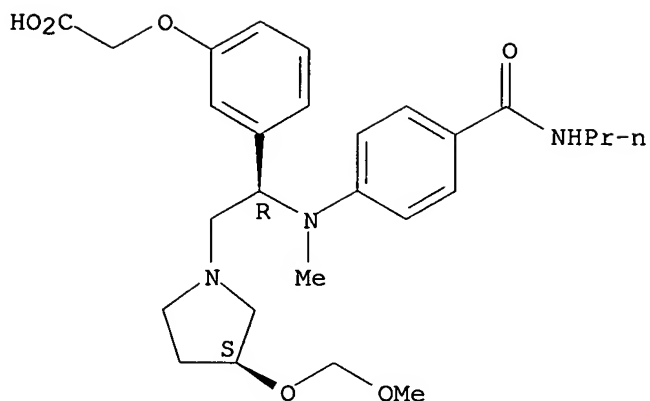


● HCl

RN 204973-57-9 CAPLUS

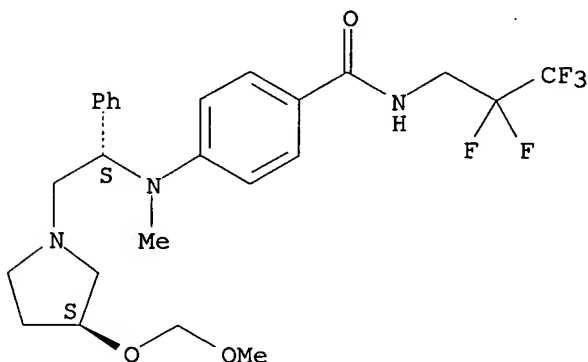
CN Acetic acid, [3-[2-[3-(methoxymethoxy)-1-pyrrolidinyl]-1-[methyl[4-[(propylamino)carbonyl]phenyl]amino]ethyl]phenoxy]-, [S-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204995-07-3 CAPLUS  
 CN Benzamide, 4-[[[(1S)-2-[(3S)-3-(methoxymethoxy)-1-pyrrolidinyl]-1-phenylethyl]methylamino]-N-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
36.38	197.92

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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 LAST RELOADED: Jan 14, 2005 (20050114/UP).

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

0.36

198.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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